

Electronic Supplementary Information

Hydrogen Adsorption on and Spillover from Au- and Cu-Supported Pt₃ and Pd₃ Clusters: A Density Functional Study

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Table S1. Properties of hydrogen adsorbed on clusters Pt₃ and Pd₃ clusters, supported on a metal or in the gas phase.^a

System	Site	$\Delta(\langle M_C-M_C \rangle)$	$\Delta(\langle M_C-M_{S1} \rangle)$	ν
Pt ₃	top	0.03	–	2238, 534, 286
	bridge	0.04	–	1541, 652, 564
	three-fold ^b	0.06	–	1418, 156, 59 <i>i</i>
Pd ₃	three-fold	0.07	–	1266, 751, 675
	bridge	0.06	–	1436, 1148, 181
Pt ₃ /Au(111)	top	0.03	–	2157, 344, 210
	rim 1	0.01	-0.01	2184, 445, 431
	bridge	0.05	-0.01	1431, 953, 396
	top ^b	0.00	0.01	2243, 255, 90 <i>i</i>
	rim 2 ^b	0.01	-0.01	1673, 1035, 288 <i>i</i>
Pd ₃ /Au(111)	three-fold	0.08	-0.02	1196, 536, 489
	three-fold	0.07	0.00	947, 879, 876
	bridge	0.04	0.01	1294, 1206, 275
	rim 2	0.01	0.00	1375, 1059, 226
	rim 1 ^b	0.01	0.00	1999, 243, 112 <i>i</i>
Pt ₃ /Cu(111)	top ^b	-0.01	0.01	1962, 135, 190 <i>i</i>
	rim 1	0.00	0.02	2074, 460, 375
	bridge	0.05	0.03	1326, 1094, 429
	three-fold	0.09	0.00	1116, 625, 595
Pd ₃ /Cu(111)	top ^b	0.00	0.02	2205, 127 <i>i</i> , 245 <i>i</i>
	three-fold	0.06	0.02	906, 900, 889
	bridge	0.03	0.03	1329, 1137, 238
	rim 3	0.02	0.00	1237, 745, 559
	top ^b	0.02	0.00	1927, 258 <i>i</i> , 284 <i>i</i>

^a Adsorption sites for hydrogen on Pt₃ and Pd₃ clusters, change Δ in the average interatomic distance $\langle M_C-M_C \rangle$ of the metal clusters after adsorption of hydrogen, change Δ in the average interatomic distance $\langle M_C-M_{S1} \rangle$ between the metal clusters and the substrate after adsorption of hydrogen, vibrational frequencies ν of adsorbed hydrogen. Distances in Å and frequency in cm⁻¹. ^b Conformation is not a local minimum, one or more imaginary frequencies.

Table S2. Properties of approximate transition states for hydrogen diffusion within metal-supported metal clusters.^a

System	Initial site	Final site	ΔE_{act}	ΔE_{diff}	$\langle M_{\text{C-H}} \rangle$	ν
Pt ₃ /Au(111)	bridge	rim 1	15	-5	1.58	2098, 304, 371 <i>i</i>
	bridge	three-fold	19	16	1.80	1304, 737, 223 <i>i</i>
Pd ₃ /Au(111)	bridge	rim 2	58	34	1.60	1661, 427, 234 <i>i</i>
	bridge	three-fold	7	-15	1.59	1860, 1167, 543 <i>i</i>
Pt ₃ /Cu(111)	bridge	rim 1	20	-18	1.59	2041, 376, 477 <i>i</i>
	bridge	three-fold	35	22	1.67	1494, 1439, 497 <i>i</i>
Pd ₃ /Cu(111)	bridge	rim 3	28	12	1.65	1374, 800, 254 <i>i</i>
	bridge	three-fold	2	-10	1.71	1328, 1094, 217 <i>i</i>

^a Initial and final sites of adsorbed hydrogen on Pt₃ and Pd₃, approximate activation energy ΔE_{act} for hydrogen diffusion from initial to final site, diffusion energy ΔE_{diff} , average nearest-neighbor distance $\langle M_{\text{C-H}} \rangle$ between atoms of the clusters and hydrogen, vibrational frequencies ν of hydrogen. Energies in kJ mol⁻¹, distances in Å, frequency in cm⁻¹.

Table S3. Properties of adsorbed hydrogen on substrate sites close to adsorbed Pt₃ and Pd₃ clusters.^a

System	Site	ΔE_{ads}	$M_{\text{C-H}}$
Pt ₃ /Au(111)	4	19	3.37
Pd ₃ /Au(111)	4	17	3.34
Pt ₃ /Cu(111)	4	-3	2.64
Pd ₃ /Cu(111)	4	-7	2.69
Pt ₃ /Au(111) ^b	1	42	2.19
	2	38	3.27
	3	14	4.69
Pt ₃ /Au(111) ^c	1	78	2.19
	2	43	3.27
	3	27	4.69

^a Adsorption sites of hydrogen on the substrate, hydrogen adsorption energy ΔE_{ads} , distance $M_{\text{C-H}}$ between adsorbed hydrogen and the nearest atom of the adsorbed cluster. Energies relative to $\frac{1}{2}\text{H}_2$ Energy in kJ mol⁻¹ and distances in Å. The distance between hydrogen and the substrate, $M_{\text{S-H}}$, was fixed to the equilibrium distances 1.75 Å for hydrogen on clean Cu(111) and 1.90 Å for hydrogen on clean Au(111). ^b Results from calculations with a six-layer slab model of the substrate. ^c Results from calculations with a (4×4) surface cell and a four-layer slab model of the substrate.

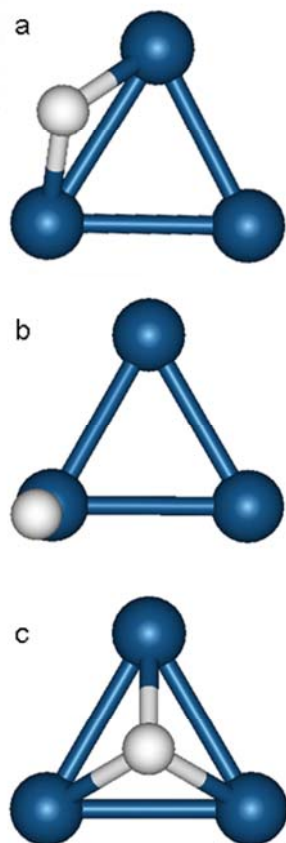


Figure S1. Sketch showing the geometries of hydrogen adsorbed on a triangular cluster: a) bridge, b) top, and c) three-fold hollow site.

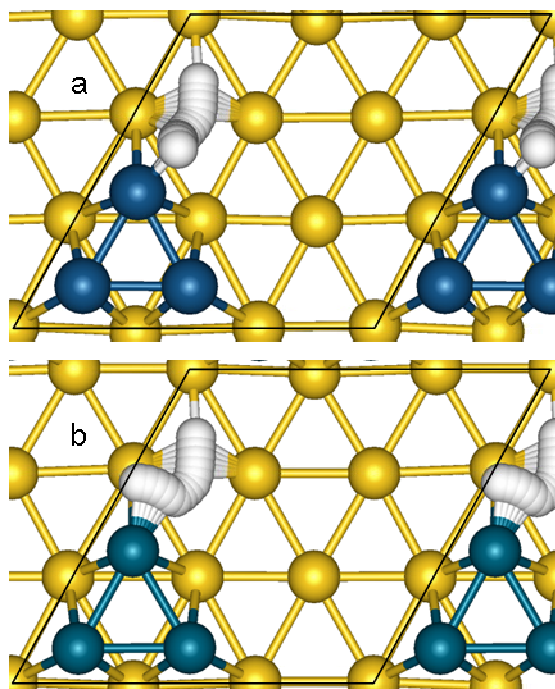


Figure S2. Hydrogen diffusion pathway from site rim 1 (Pt_3) and rim 2 (Pd_3) to site 4 on a) $\text{Pt}_3/\text{Au}(111)$ and b) $\text{Pd}_3/\text{Au}(111)$.

Cartesian Coordinates of Stationary Points

Cartesian coordinates of all systems studied are listed as they appear in the tables of the main document.

The two “bottom” atomic layers of the surface models kept fixed during geometry optimization are included separately (au_2fixed_layers, cu_2fixed_layers). Only the two top-most optimized layers of the surfaces are include for each system.

1	Table 1	S7
1.1	pt3_gas	S7
1.2	pt3_gas-h_top	S7
1.3	pt3_gas-h_bridge	S7
1.4	pt3_gas-h_three-fold	S7
1.5	pd3_gas	S7
1.6	pd3_gas-h_three-fold	S7
1.7	pd3_gas-h_bridge	S7
1.8	pd3_gas_top	S7
1.9	au_2fixed_layers	S7
1.10	pt3_au	S7
1.11	pt3_au-h_rim1	S8
1.12	pt3_au-h_bridge	S8
1.13	pt3_au-h_top	S8
1.14	pt3_au-h_rim2	S9
1.15	pt3_au-h_three-fold	S9
1.16	pd3_au	S9
1.17	pd3_au-h_three-fold	S10
1.18	pd3_au-h_bridge	S10
1.19	pd3_au-h_rim2	S10
1.20	pd3_au-h_rim1	S11
1.21	pd3_au-h_top	S11
1.22	cu_2fixed_layers	S11
1.23	pt3_cu	S12
1.24	pt3_cu-h_rim1	S12
1.25	pt3_cu-h_bridge	S12
1.26	pt3_cu-h_three-fold	S13
1.27	pt3_cu-h_top	S13
1.28	pd3_cu	S13
1.29	pd3_cu-h_three-fold	S14
1.30	pd3_cu-h_bridge	S14
1.31	pd3_cu-h_rim3	S14
1.32	pd3_cu-h_top	S15
2	Table 2	S16
2.1	pt3_au-h_au-site1	S16
2.2	pt3_au-h_au-site2	S16
2.3	pt3_au-h_au-site3	S16
2.4	pd3_au-h_au-site1	S17
2.5	pd3_au-h_au-site2	S17

2.6	pd3_au-h_au-site3	S17
2.7	pt3_cu-h_cu-site1	S18
2.8	pt3_cu-h_cu-site2	S18
2.9	pt3_cu-h_cu-site3	S18
2.10	pd3_cu-h_cu-site1	S19
2.11	pd3_cu-h_cu-site2	S19
2.12	pd3_cu-h_cu-site3	S19
2.13	au-h_fcc	S20
2.14	cu-h_fcc	S20
3	Table 3.....	S21
3.1	pt3_au-h_rim1_to_au-site4_TS	S21
3.2	pd3_au-h_rim2_to_au-site4_TS	S21
3.3	pt3_cu-h_rim1_to_cu-site4_TS	S21
3.4	pd3_cu-h_rim3_to_cu-site4_TS	S22
4	Table S2.....	S23
4.1	pt3_au-h_bridge_to_rim1_TS	S23
4.2	pt3_au-h_bridge_to_three-fold_TS	S23
4.3	pd3_au-h_bridge_to_rim2_TS.....	S23
4.4	pd3_au-h_bridge_to_three-fold_TS	S24
4.5	pt3_cu-h_bridge_to_rim1_TS	S24
4.6	pt3_cu-h_bridge_to_three-fold_TS	S24
4.7	pd3_cu-h_bridge_to_rim3_TS.....	S25
4.8	pd3_cu-h_bridge_to_three-fold_TS	S25
5	Table S3.....	S26
5.1	pt3_au-h_au-site4	S26
5.2	pd3_au-h_au-site4	S26
5.3	pt3_cu-h_cu-site4	S26
5.4	pd3_cu-h_cu-site4	S27
5.5	pt3_au_6layers.....	S27
5.6	pt3_au_6layers-h_au-site1	S28
5.7	pt3_au_6layers-h_au-site2.....	S28
5.8	pt3_au_6layers-h_au-site3.....	S28
5.9	pt3_au4x4	S29
5.10	pt3_au4x4-h_au-site1	S30
5.11	pt3_au4x4-h_au-site2	S30
5.12	pt3_au4x4-h_au-site3	S31

1 Table 1

<i>1.1 pt3_gas</i>			
Pt	9.40318760843739	7.15688715126569	12.55000000000008
Pt	10.64855924108518	4.99982907564507	12.55000000000008
Pt	8.15780715047737	4.99982377308924	12.55000000000008
<i>1.2 pt3_gas-h_top</i>			
H	7.92854298930410	4.87178614620980	13.95195141126165
Pt	9.35617218713125	7.22824773246165	12.11921243249094
Pt	10.68357438780149	4.92929603914049	12.11757288185060
Pt	8.07923254161892	4.95828425750443	12.39976796095789
<i>1.3 pt3_gas-h_bridge</i>			
H	1.28571292580108	-0.36184093598323	1.14433591027688
Pt	0.00000000000000	0.00000000000000	0.00000000000000
Pt	2.54378872106259	0.00000000000000	0.00000000000000
Pt	1.27263369079887	2.17762072007048	0.00000000000000
<i>1.4 pt3_gas-h_three-fold</i>			
H	1.27300000000002	0.74400000000003	1.07709983049825
Pt	0.00000000000000	0.00000000000000	0.00000000000000
Pt	2.55177360641509	0.00000000000000	0.00000000000000
Pt	1.26939088511478	2.21158141762700	0.00000000000000
<i>1.5 pd3_gas</i>			
Pd	4.01324600000001	4.78967727863592	1.88001900000003
Pd	5.26501452476648	2.61344786068207	1.88001900000003
Pd	2.76146847523347	2.61344286068208	1.88001900000003
<i>1.6 pd3_gas-h_three-fold</i>			
H	1.27300000000002	0.74400000000003	0.99398291274336
Pd	0.00000000000000	0.00000000000000	0.00000000000000
Pd	2.57716552561074	0.00000000000000	0.00000000000000
Pd	1.28012494293159	2.23065383919390	0.00000000000000
<i>1.7 pd3_gas-h_bridge</i>			
H	8.44877708774088	6.26954734905125	13.23167096486370
Pd	9.20578992833684	7.33348043483416	12.16540459655219
Pd	10.50075355205223	5.13869349175684	12.10276960339952
Pd	7.95343838572079	5.05264152948502	12.17553217669437
<i>1.8 pd3_gas_top</i>			
H	0.00000000000000	0.00000000000000	1.51734995877727
Pd	0.00000000000000	0.00000000000000	0.00000000000000
Pd	2.53844984310741	0.00000000000000	0.00000000000000
Pd	1.26315746486398	2.20010156709611	0.00000000000000
<i>1.9 au_2fixed_layers</i>			
Au	10.87900700000000	4.86678000000002	5.32010000000004
Au	4.97582700000000	4.86676900000000	5.32010000000004
Au	9.40320800000002	2.31061899999998	5.32010000000004
Au	6.45157400000000	2.31063900000000	5.32010000000004
Au	7.92737400000002	4.86679999999998	5.32010000000004
Au	3.50002699999999	2.31060800000002	5.32010000000004
Au	12.35480900000002	7.42294100000000	5.32010000000004
Au	9.40317300000000	7.42296000000001	5.32010000000004
Au	6.45162700000002	7.42292999999998	5.32010000000004
Au	7.92736799999998	1.45858900000001	2.91009999999997
Au	10.87896700000004	6.57091000000002	2.91009999999997
Au	6.45162100000004	4.01471900000002	2.91009999999997
Au	4.97578600000004	6.57090000000001	2.91009999999997
Au	9.40316799999999	4.01474999999999	2.91009999999997
Au	4.97582099999999	1.45855899999999	2.91009999999997
Au	2.02418599999998	1.45857800000000	2.91009999999997
Au	7.92742099999999	6.57088000000000	2.91009999999997
Au	3.49998699999999	4.01473899999998	2.91009999999997
<i>1.10 pt3_au</i>			
Pt	9.41000567537797	7.23846706688116	12.20532326549838
Pt	10.72118078025244	4.97176118567258	12.20717618361868
Pt	8.10538858983690	4.97157228333583	12.20405314290107
Au	7.92980864603329	1.46272694906535	10.13317784144126
Au	4.97882770047342	6.57200594885900	10.13346822108581
Au	4.97956911168102	1.53165050424642	10.30464027152979
Au	6.40461528394440	3.98835977781809	10.30654175234542
Au	11.01110797933591	6.65175471280656	10.04950799879210

Au	9.41223055871118	3.87177892827019	10.04910856391772
Au	2.02457373999724	1.45931329284689	10.13091953471050
Au	7.80598885226248	6.65066496651894	10.04722158559325
Au	3.56216517626263	3.98934754729607	10.30568717139095
Au	6.43494705885043	0.61642347199435	7.71288058418509
Au	9.40141458722578	5.71827701902447	7.72832372670553
Au	3.49879704420908	5.70148989422936	7.71396037348655
Au	4.97662153287733	3.16610780886085	7.79105958777095
Au	7.91287869383096	3.16899133017057	7.71473937233205
Au	3.51459659911758	0.61882526645098	7.71282454513785
Au	0.54583619293272	0.60594295352603	7.70932818180753
Au	6.44892284011308	5.70132784317698	7.71421274301878
Au	2.04092974757702	3.17237578084701	7.71395407271568
<i>1.11 pt3_au-h_rim1</i>			
H	6.62622670906057	5.34328402397803	12.78846172566860
Pt	9.41331712359191	7.27530056793345	12.19485188830209
Pt	10.70407974178066	4.99953943303764	12.16450486561723
Pt	8.04712384756374	5.02024024828793	12.19069473850714
Au	7.95581663244760	1.49037346288141	10.13868826089229
Au	5.00751420211028	6.62564634574682	10.11053121814071
Au	5.00292004096868	1.56115055106705	10.30551562223405
Au	6.40181076087876	4.01159097167805	10.27834351936242
Au	11.03369714056492	6.68322672705583	10.04310937908988
Au	9.42321896230352	3.89291813642643	10.03405274905984
Au	2.05190455622012	1.49580483399886	10.16359427588196
Au	7.84223002009252	6.68605034374609	10.02076896545781
Au	3.55158101790307	4.00818201766610	10.28579139500390
Au	6.45733217995809	0.63616101403954	7.70731511091342
Au	9.42701520307449	5.73846049159026	7.71899207374708
Au	3.53108549962472	5.71953198966028	7.71245881340259
Au	4.99441859643025	3.18860073304051	7.79656954672452
Au	7.93173037268659	3.18643672078713	7.71227154578364
Au	3.53273368534457	0.64474978118818	7.70620770778577
Au	0.57389256859172	0.63452111970071	7.70873698302028
Au	6.47496715363659	5.71618883147200	7.70844679581668
Au	2.06265699388969	3.18746717503238	7.69857714950467
<i>1.12 pt3_au-h_bridge</i>			
H	8.08685997652059	6.47455048077105	13.11602877705511
Pt	9.33116447023134	7.32375549678283	12.23780353838010
Pt	10.67087665698953	5.02847836854905	12.07971362588672
Pt	8.01985785010922	4.96757845902435	12.24183140018866
Au	7.94394477861773	1.47324388832260	10.15521791175976
Au	4.96053955181115	6.58062590285137	10.14534089048016
Au	4.98899717368345	1.55303796274551	10.29006520685000
Au	6.39988246351926	3.99447811595427	10.28102928976832
Au	10.97266864794395	6.72201889964084	10.02250914448043
Au	9.36989763925673	3.87344968547199	10.02652832406227
Au	2.02913113518678	1.46980127281678	10.14473069752843
Au	7.81619827576421	6.63899698784995	10.04264505117409
Au	3.55577468723638	4.00173823231178	10.30405777496602
Au	6.44745490303166	0.63672927914945	7.69804157347379
Au	9.41117519783769	5.72064145500375	7.71656434956210
Au	3.50242355277403	5.70253210435048	7.71347527707008
Au	4.97499128688551	3.17718905788003	7.78651814190335
Au	7.91367004551107	3.16919268744897	7.70296429229469
Au	3.52676735669868	0.62361126701884	7.72115686587451
Au	0.55449295572483	0.60635325944308	7.72298815935753
Au	6.45352580306366	5.70582504462041	7.71842015627629
Au	2.05387281147419	3.16884180901933	7.70813898487632
<i>1.13 pt3_au-h_top</i>			
H	7.92854298930412	4.87178614620982	13.95195141126162
Pt	9.35617218713125	7.22824773246164	12.11921243249101
Pt	10.68357438780150	4.92929603914049	12.11757288185066
Pt	8.07923254161891	4.95828425750445	12.39976796095798
Au	7.93804232824591	1.46015234680945	10.13861856964490
Au	4.97828757003566	6.58243030896856	10.13864724852342
Au	5.00452558306512	1.54993694298054	10.30725010794107
Au	6.43184692692808	4.00783710267767	10.35912986149465
Au	11.02622683901784	6.66051069748036	10.02876538608240

Au	9.34057882458148	3.89189130169013	10.04333961336867
Au	2.04666905268162	1.47915083402677	10.13929157502483
Au	7.78434281457742	6.58928754963018	10.04471960630561
Au	3.59003603922458	3.99504014567981	10.30952881769364
Au	6.44173855332294	0.62448948802737	7.70416599567493
Au	9.40649843372581	5.72418935941503	7.72393003690062
Au	3.50681151523591	5.70420469918010	7.70452987863441
Au	4.98768588247557	3.17384513213829	7.80257493573971
Au	7.91381752204461	3.17067721270434	7.71045516029403
Au	3.52855394968721	0.63624121415872	7.71949189504844
Au	0.55890267779229	0.61314276784606	7.71982980584996
Au	6.45191018930739	5.70376041029879	7.71062567434306
Au	2.05911221771227	3.17835198064146	7.71852669235489
<i>1.14 pt3_au-h_rim2</i>			
H	6.66601500000002	4.09951799999999	12.05902600000005
Pt	9.41360300000001	7.27168900000002	12.19545300000004
Pt	10.70496700000000	5.00149100000001	12.16769000000002
Pt	8.04945099999999	5.01887399999999	12.19397500000004
Au	7.95461400000001	1.49273899999998	10.13723600000006
Au	5.00687300000000	6.62482599999999	10.11008999999999
Au	5.00305900000002	1.56111700000001	10.30509699999995
Au	6.40244000000003	4.01409400000002	10.27844999999999
Au	11.03425499999998	6.68530299999998	10.04056399999995
Au	9.42454799999998	3.89402100000000	10.03348399999999
Au	2.05178300000000	1.49586300000002	10.16065300000001
Au	7.84077499999998	6.68648900000001	10.01938199999995
Au	3.55103699999998	4.01088399999998	10.28500900000003
Au	6.45757400000002	0.63721100000001	7.70752099999999
Au	9.42614000000000	5.73865399999999	7.71829599999998
Au	3.53006999999997	5.72040599999998	7.71182300000001
Au	4.99422799999998	3.18859900000002	7.79706899999999
Au	7.93255499999999	3.18822099999999	7.71147700000005
Au	3.53168199999999	0.64549600000002	7.70677500000005
Au	0.57326900000000	0.63559600000002	7.70829300000008
Au	6.47339100000000	5.71749799999999	7.70786599999994
Au	2.06268999999998	3.18712400000003	7.69734700000001
<i>1.15 pt3_au-h_three-fold</i>			
H	9.40649014825242	5.75862160394383	13.18770867883610
Pt	9.41148581562959	7.30996371789543	12.17023165789177
Pt	10.76597117797414	4.96095771037831	12.17312072169577
Pt	8.05709011617537	4.95939976544615	12.17541430024638
Au	7.92987438753211	1.46832802505286	10.14411212184074
Au	4.97990300931179	6.57261155555992	10.14597771841318
Au	4.98168799221974	1.54661112797947	10.27421825534793
Au	6.39908033831190	3.98938784155667	10.28926687312550
Au	11.00935577393682	6.65721148065780	10.04169708894125
Au	9.41014067726137	3.87876437973456	10.05145444625779
Au	2.02648579650464	1.46590492140047	10.14039149116244
Au	7.80972898307848	6.65558710846812	10.04267302488918
Au	3.56833617672877	3.98988912074600	10.28928183774985
Au	6.43471150330456	0.62221927823208	7.71086041422071
Au	9.40158756135717	5.72084990778204	7.72651556798637
Au	3.50057604050687	5.70275840235527	7.71407938810158
Au	4.97579094074130	3.16943875965243	7.76902558756191
Au	7.91163005418982	3.17168016976575	7.71642495469299
Au	3.51560912635056	0.62433946929678	7.71174775401353
Au	0.54572650290654	0.60673874306111	7.72084439128813
Au	6.44961026592307	5.70249329860622	7.71557660584714
Au	2.04129294201148	3.17601366901201	7.71532424448278
<i>1.16 pd3_au</i>			
Pd	9.41516311924113	7.30955143340923	12.19345048945281
Pd	10.78154809860251	4.94456320502350	12.19333294191404
Pd	8.05203632749597	4.94440431704768	12.19441138445110
Au	7.94424092835866	1.45812166981507	10.13890140189447
Au	4.98085068891614	6.59358401328882	10.14101157502433
Au	4.98499554992078	1.52466972299977	10.20063387244499
Au	6.41344449863187	3.99790332153412	10.20133084191256
Au	10.97190450522499	6.62843288048769	10.07403187406776
Au	9.41343422107872	3.91893877318161	10.07883131718640

Au	2.01692204667674	1.45569859073270	10.13418802759888
Au	7.84860826065293	6.63075027155278	10.07701079931055
Au	3.55833592857953	3.99427023421483	10.20082396361105
Au	6.44352761690105	0.61124994056254	7.71453159381468
Au	9.40200896448352	5.71984662738668	7.71724778468732
Au	3.49885884915261	5.71228422089577	7.71455474925508
Au	4.97745333119143	3.16496123046842	7.73260927697047
Au	7.92151745010193	3.17112039381772	7.71672829490649
Au	3.50997495114958	0.61271176457321	7.71310633201614
Au	0.54664679861020	0.60740321023110	7.70821154109990
Au	6.45325233695139	5.71365991849361	7.71661518637292
Au	2.03160399960690	3.17102656840621	7.71427836558166
<i>1.17 pd3_au-h_three-fold</i>			
H	9.41703584591367	5.74861311167590	13.01412174648739
Pd	9.41591568767322	7.36517715936847	12.20920877967766
Pd	10.81885151345632	4.93595781030258	12.21479588357140
Pd	8.01466704033414	4.93534757074827	12.21383168143978
Au	7.93455644012837	1.46814684225614	10.13732023387961
Au	4.97952180974377	6.57911722212550	10.13807090437833
Au	4.98548636263441	1.53754673718682	10.18202577326434
Au	6.41158003709350	3.99958864693592	10.19078526898065
Au	10.97230535406553	6.63639808840193	10.09038946517592
Au	9.41252153203214	3.92324001596624	10.10075054908237
Au	2.02430552634757	1.46670743874690	10.13335048860605
Au	7.84541106281623	6.64071498354452	10.09420402715425
Au	3.55948744687803	3.99625199431651	10.19274985731731
Au	6.44089462480558	0.61112792246203	7.71958882036024
Au	9.40167524168280	5.72387462300663	7.72131574807535
Au	3.49289778714273	5.71373243009535	7.72170076835765
Au	4.97609731775696	3.16956257366205	7.70332794846155
Au	7.92385158204400	3.17827341294222	7.72340435472012
Au	3.51175067138104	0.61362139625965	7.71992974117970
Au	0.54676944691633	0.60935340112997	7.71577021004246
Au	6.45766083144425	5.71514969761541	7.72260720903597
Au	2.02795617817933	3.17979772009863	7.72266809528251
<i>1.18 pd3_au-h_bridge</i>			
H	8.08685997652062	6.47455048077107	12.99000966670450
Pd	9.30536973507877	7.39337463792569	12.25299497533810
Pd	10.69470184925889	5.01500240301981	12.14984729535876
Pd	7.94118701743765	4.96354963636232	12.25075830916822
Au	7.93822885071458	1.48243475658346	10.14370277446253
Au	4.95948619326527	6.59010915364602	10.13438819389440
Au	4.97232338571061	1.54619401817725	10.18771464298308
Au	6.39483119208339	4.00450621191766	10.18356233054084
Au	10.94617825227775	6.70268101303884	10.08243032815595
Au	9.36687502102635	3.92578746909357	10.08186805945012
Au	2.02031464624070	1.47969643617790	10.13924737530287
Au	7.84483363327091	6.62724919174552	10.07042121935862
Au	3.52359595006000	4.01991862245818	10.21995121050605
Au	6.44727114102371	0.62352246563755	7.70771474912087
Au	9.41401235922523	5.72494104782156	7.72226568941529
Au	3.49663442684501	5.71583687834756	7.71952754182264
Au	4.96839715775898	3.17720113602519	7.72698564242476
Au	7.92490456737466	3.17869273826994	7.71061139985302
Au	3.51314310232403	0.61605936560626	7.72101206509299
Au	0.55253720369687	0.61362458802621	7.71577643184209
Au	6.45478467417408	5.71670563630909	7.71915563351973
Au	2.03903673848402	3.17885965197485	7.71723235054512
<i>1.19 pd3_au-h_rim2</i>			
H	6.63090825399857	4.35327398857327	12.00709208536223
Pd	9.50448156866995	7.44277709023990	12.21846463340165
Pd	10.87697235862196	5.08989500885429	12.22026337893004
Pd	8.14130534163020	5.05483984601934	12.18382338220039
Au	7.97389009818125	1.54816717216482	10.12830001425658
Au	5.00749161216617	6.68882073248148	10.12141079349492
Au	4.99327245584173	1.57818051136664	10.16281286756220
Au	6.38589766226576	4.06325450153729	10.24814138562672
Au	11.00809056388680	6.72413766682922	10.06939879638974
Au	9.47292739714597	3.99338227595737	10.10393726564127

Au	2.04505447208233	1.53487750515158	10.13633432368656
Au	7.89190380364102	6.73251008049452	10.09456205671120
Au	3.53821154792714	4.07836674353060	10.16746951098020
Au	6.46986294104306	0.67480096941904	7.70231755728947
Au	9.42341186011057	5.77493042607887	7.72814249245811
Au	3.52379835438438	5.77332015714437	7.70515978361930
Au	5.01378213550323	3.23619208362913	7.75280569137450
Au	7.94353964660315	3.24041003521709	7.73671299876605
Au	3.52625175398312	0.66301274040802	7.70030629241876
Au	0.57173366884819	0.66772602908979	7.70062295879915
Au	6.48350075467458	5.76868868348759	7.73057411653403
Au	2.04590437122131	3.22290488900350	7.70109360226696
<i>1.20 pd3_au-h_rim1</i>			
H	6.74090999999997	5.17327399999999	12.82710600000000
Pd	9.50448099999999	7.44277700000000	12.21846500000002
Pd	10.87697199999999	5.08989499999999	12.22026300000006
Pd	8.14130500000001	5.05484000000001	12.18382400000006
Au	7.97389000000002	1.54816700000000	10.12829999999999
Au	5.00749200000001	6.68882099999998	10.12141000000003
Au	4.99327200000003	1.57818100000001	10.16281299999999
Au	6.38589799999997	4.06325400000000	10.24814100000000
Au	11.00809100000001	6.72413800000002	10.06939900000006
Au	9.47292700000004	3.99338200000002	10.10393700000005
Au	2.04505400000001	1.53487799999999	10.13633400000003
Au	7.89190400000004	6.73251000000003	10.09456299999994
Au	3.53821199999999	4.07836700000002	10.16747000000007
Au	6.46986299999998	0.67480099999998	7.70231799999992
Au	9.42341200000000	5.77493000000000	7.72814199999996
Au	3.52379800000001	5.77331999999998	7.70516000000005
Au	5.01378199999996	3.23619199999998	7.75280599999996
Au	7.94354000000002	3.24041000000002	7.73671300000008
Au	3.52625199999998	0.66301300000002	7.70030600000003
Au	0.57173400000000	0.66772600000000	7.70062300000005
Au	6.48350100000004	5.76868900000002	7.73057400000005
Au	2.04590399999997	3.22290499999998	7.70109399999998
<i>1.21 pd3_au-h_top</i>			
H	8.07923254161892	4.95828425750443	13.80821096293195
Pd	9.29179506435600	7.24665442176949	12.19733835784162
Pd	10.66493209876828	4.86607710243854	12.19778355530539
Pd	7.95589785941671	4.89120288249528	12.25827288295151
Au	7.92423184521562	1.44724119950605	10.13324381815536
Au	4.95782910051148	6.58983579707655	10.13506374816702
Au	4.97192918081115	1.50968989590046	10.22475910003558
Au	6.39678533228082	3.98989906962324	10.17580840794494
Au	10.95428862486741	6.62368683826518	10.12038107092933
Au	9.35525638352264	3.91444157894679	10.05294773748369
Au	2.02491105904230	1.47053107016395	10.13426085592100
Au	7.80721005741086	6.59576282304405	10.05468996962431
Au	3.53769709510559	3.99918699047512	10.22877403097677
Au	6.43693971099646	0.60385774999545	7.72284572653237
Au	9.40257893680043	5.72585434399543	7.72257376077136
Au	3.48792416920551	5.71442768389895	7.72449197124789
Au	4.96469018559489	3.16070980444248	7.73305410780085
Au	7.91322541528830	3.16459468370203	7.70462027547023
Au	3.51310448867544	0.62360222388603	7.71513798069088
Au	0.55121678644858	0.61305332961710	7.71477163229011
Au	6.44322046264209	5.71172586889850	7.70466974842004
Au	2.04047984727841	3.17806566840644	7.71597989500445
<i>1.22 cu_2fixed_layers</i>			
Cu	9.49630347615275	4.24822043332364	4.64392422244793
Cu	4.34340774271353	4.24821083140515	4.64392422244793
Cu	8.20807605118625	2.01694320462929	4.64392422244793
Cu	5.63158977679275	2.01696066266288	4.64392422244793
Cu	6.91981807466096	4.24823789135718	4.64392422244793
Cu	3.05517944484532	2.01693360271085	4.64392422244793
Cu	10.78453351982433	6.47949766201794	4.64392422244793
Cu	8.20804549962747	6.47951424714985	4.64392422244793
Cu	5.63163604058175	6.47948806009946	4.64392422244793
Cu	6.91981283725085	1.27320478707094	2.54023117605788

Cu	9.49626856008563	5.73575837155791	2.54023117605788
Cu	5.63163080317169	3.50445495581321	2.54023117605788
Cu	4.34337195374473	5.73574964254111	2.54023117605788
Cu	8.20804113511907	3.50448201576524	2.54023117605788
Cu	4.34340250530345	1.27317860002055	2.54023117605788
Cu	1.76691535800827	1.27319518515246	2.54023117605788
Cu	6.91985910103985	5.73573218450752	2.54023117605788
Cu	3.05514452877817	3.50447241384676	2.54023117605788
<i>1.23 pt3_cu</i>			
Pt	4.34851866569533	-0.14760653729969	10.78824622610841
Pt	9.55568570261095	4.22406528768064	10.78909427562627
Pt	6.87245141001855	4.22276164891639	10.79002691664485
Cu	6.90583933928697	1.28520576853599	8.92818519323081
Cu	4.34552634846998	5.71911115427403	8.92884064441137
Cu	4.34560227040404	1.32746499304153	8.78881662853581
Cu	5.58982140922789	3.48136091360396	8.79289906049773
Cu	9.56719767130257	5.77828361973573	8.78215756613219
Cu	8.21181134859693	3.42847246781541	8.78499721386643
Cu	1.78520897109880	1.28461709373527	8.92670766584788
Cu	6.85478262070671	5.77834512785260	8.78426071939604
Cu	3.10187358716582	3.48102039746850	8.79024278402502
Cu	5.64205346786353	0.53197768528848	6.73288221527628
Cu	8.20957110939696	4.99375055922216	6.72510155020074
Cu	3.06163830174113	5.00095792036322	6.73334778345788
Cu	4.34500400105290	2.76281148944872	6.70167919018622
Cu	6.92509132856998	2.75396043238425	6.73485816025123
Cu	3.04693798680680	0.53185501464339	6.73334051576908
Cu	0.47914826145520	0.53044981584761	6.82668464761276
Cu	5.62748192691739	5.00116330089382	6.73466288130306
Cu	1.76412449577178	2.75374224440750	6.73370696456937
<i>1.24 pt3_cu-h_rim1</i>			
H	5.32035369760553	4.43351317402775	11.15482361327895
Pt	4.47021002510083	-0.10599187134155	10.78970278433612
Pt	9.54714368212223	4.21483981638089	10.80291112501886
Pt	6.87372582267304	4.32254439564460	10.81994217772442
Cu	6.90387835618624	1.26931883688908	8.93225296903732
Cu	4.38053055697775	5.73286259766751	8.90572005967560
Cu	4.35072281161131	1.33679947793231	8.77537062040927
Cu	5.60406174712919	3.48258170445043	8.83109542024062
Cu	9.59871626175221	5.75778340395087	8.76722756724974
Cu	8.21457694227143	3.42419518396114	8.79147244290187
Cu	1.78420778335637	1.29325345907712	8.90239278853704
Cu	6.90216303714230	5.81266488519588	8.78884338121744
Cu	3.09457284085481	3.48217766991869	8.78753840396992
Cu	5.64459114944623	0.52560147440994	6.72842308038580
Cu	8.21505234745723	4.98982484167142	6.72705509575494
Cu	3.07799639292660	4.99733190779463	6.72895314700686
Cu	4.35589244338593	2.77130654129404	6.71094591084102
Cu	6.92728086898849	2.75229374920666	6.74724224673395
Cu	3.05185409618426	0.53173165359315	6.72657203437962
Cu	0.48000171178160	0.53005779804151	6.82065830494915
Cu	5.64376139084525	4.99871029925301	6.74839171861249
Cu	1.76765706850615	2.75464291690458	6.72598191060799
<i>1.25 pt3_cu-h_bridge</i>			
H	6.85150984248137	5.78199867559204	11.38357118919490
Pt	4.43036967287468	-0.11893725333827	10.84628382208667
Pt	9.56250512034486	4.21659017754805	10.74303048988038
Pt	6.88528863683718	4.13393351412292	10.84724444647109
Cu	6.90182642259573	1.28401698850575	8.94856535439062
Cu	4.33924875889325	5.72309827531809	8.90932469326970
Cu	4.34718033172664	1.32386612118883	8.80337475373502
Cu	5.59208151025801	3.47768740906494	8.80588646913022
Cu	9.56154359837136	5.77459887814783	8.74970000242613
Cu	8.20903374512082	3.43060479735045	8.75218561859436
Cu	1.77541479936690	1.28443143034383	8.90754135667759
Cu	6.88277159195107	5.76019856958323	8.82439716079763
Cu	3.11432120655782	3.47155127888662	8.76934074047033
Cu	5.63918017128214	0.53323301783392	6.73399270235072
Cu	8.20717192983149	4.99250221266056	6.71561375895602

Cu	3.06594028439906	4.99501581275238	6.72189894005407
Cu	4.35075165321191	2.75700238271427	6.69902934094844
Cu	6.92066083031582	2.75118661785113	6.73525554771722
Cu	3.04972567483083	0.52438897179176	6.75256822053070
Cu	0.47453311199339	0.53060092976319	6.82849279408151
Cu	5.63367001465915	4.99917336046386	6.75346886091604
Cu	1.76962227145955	2.74962874102314	6.72259812403729
<i>1.26 pt3_cu-h_three-fold</i>			
H	8.21345542789067	5.00596802064071	11.73084182848475
Pt	4.34950090603994	-0.09458412076182	10.78298948632031
Pt	9.59789433878458	4.20333833249494	10.78476991620401
Pt	6.83143506931768	4.20177224695384	10.78614848107707
Cu	6.90099556761708	1.28876892055611	8.93445021574153
Cu	4.34558677254353	5.71396474846983	8.93519808457534
Cu	4.34615557634591	1.34131018532115	8.75419519076981
Cu	5.57956586380501	3.47633536741685	8.76227992521317
Cu	9.56174658595447	5.77634537019736	8.78816063978563
Cu	8.21203325126539	3.43564077778832	8.79281706159405
Cu	1.79045716460183	1.28814529853697	8.93252271532843
Cu	6.86083599865456	5.77630453098788	8.79109300321137
Cu	3.11274022295971	3.47535034116260	8.75872760352417
Cu	5.64357890565574	0.53036679387528	6.73233904089569
Cu	8.20948243334604	4.99388282730478	6.72709118530833
Cu	3.06079187828946	5.00325661266391	6.73350405825188
Cu	4.34516834841986	2.76356127709920	6.67064782848180
Cu	6.92724246622142	2.75406959698064	6.73545420091424
Cu	3.04551589907633	0.53029045425836	6.73294265699864
Cu	0.47913246412654	0.53100519955810	6.83721439939882
Cu	5.62834701584044	5.00367849699555	6.73498811057086
Cu	1.76182697470388	2.75393231646059	6.73422249773176
<i>1.27 pt3_cu-h_top</i>			
H	6.87271793859643	4.31582946889368	12.38294080510269
Pt	8.32773218032541	6.58855283717456	10.79073783332429
Pt	9.54509772644006	4.21802563633645	10.80456496405003
Pt	6.87271777192606	4.31582918177583	10.81545988384498
Cu	6.90330754659212	1.26805225605835	8.93160318001446
Cu	4.37840192194916	5.73310229275355	8.90337370443301
Cu	4.34943099126058	1.33561351335029	8.77520509801888
Cu	5.59982267509599	3.48153654330904	8.83120701362264
Cu	9.59275195604776	5.75696975783187	8.76672339771608
Cu	8.21434882564594	3.42602161404126	8.78880693956398
Cu	1.78487984962366	1.29460206666442	8.90395505639668
Cu	6.90121740469817	5.81155673108048	8.78835144696497
Cu	3.08918721415225	3.48185779898475	8.788737326370142
Cu	5.64378279355669	0.52668920814454	6.72833874248062
Cu	8.21368412612368	4.98918510636419	6.72261761424722
Cu	3.07776381214237	4.99594912926890	6.72778360574734
Cu	4.35416114750686	2.77109791918744	6.71193056125494
Cu	6.92465601861363	2.75092450186453	6.74733102138520
Cu	3.05209645699388	0.53250231732419	6.72672313227704
Cu	0.48020684367826	0.52910988167471	6.82214708010522
Cu	5.64228367914630	4.99770183698795	6.74870542408005
Cu	1.76614000191995	2.75412794045260	6.72501348853354
<i>1.28 pd3_cu</i>			
Pd	8.21624657690941	6.58507956695830	10.82304649807667
Pd	9.59078227377986	4.20631918629339	10.82410398642530
Pd	6.84150557302312	4.20497255802834	10.82460600163159
Cu	6.91361335047862	1.28174747941337	8.89794121484011
Cu	4.34608621825145	5.72841652253090	8.89824176233558
Cu	4.34583564322121	1.31552710153428	8.77364501541873
Cu	5.60115817089274	3.48827235427580	8.77737463585670
Cu	9.54208903822594	5.76357154652103	8.81129238810060
Cu	8.21297523606350	3.45995827933180	8.81446113605109
Cu	1.77759825259138	1.28067143816650	8.89643093243961
Cu	6.88220079677954	5.76397667538950	8.81360968692202
Cu	3.09171649458869	3.48743567109975	8.77458704486182
Cu	5.64090089110338	0.52845637052268	6.73529940905471
Cu	8.20934542146408	4.99378428866660	6.73183472201447
Cu	3.05796592378600	5.00204358338510	6.73550632155262

Cu	4.34497853705363	2.76285285475816	6.69839692268459
Cu	6.92756433073796	2.75655640292718	6.73710067850737
Cu	3.04769381297086	0.52854166792347	6.73569140231645
Cu	0.47889399427356	0.53059778169446	6.80256554585777
Cu	5.63076449220698	5.00233338814252	6.73704351267621
Cu	1.76148081000756	2.75644426544294	6.73594864430192
<i>1.29 pd3_cu-h_three-fold</i>			
H	8.21416290685091	5.00423226495576	11.63444808697358
Pd	4.34959861902084	-0.06984586723814	10.83863415938323
Pd	9.61912014486997	4.19255629449921	10.84044823596854
Pd	6.81068927979740	4.19112155005112	10.84107079398765
Cu	6.90758680162330	1.28563481431801	8.89426300736354
Cu	4.34603553158163	5.72126049333496	8.89496007513545
Cu	4.34572276123296	1.33006783894352	8.74443383807981
Cu	5.58890709947675	3.48169242328469	8.75050829843610
Cu	9.53794735693413	5.76297096104290	8.82257053502950
Cu	8.21238096233226	3.464456913221151	8.82618525994249
Cu	1.78372216353901	1.28435101673355	8.89281928397511
Cu	6.88612459588474	5.76269603299628	8.82432750121616
Cu	3.10275978245509	3.48109143119903	8.74829311294966
Cu	5.64303497890044	0.52561341488087	6.73705872928119
Cu	8.20949478130432	4.99398092823321	6.73768638603409
Cu	3.05631017186332	5.00534098237828	6.73811258239762
Cu	4.34483841308913	2.76339031828939	6.67189627609762
Cu	6.93107440152695	2.75680261668075	6.73959116329699
Cu	3.04586067145158	0.52566466243678	6.73736758637836
Cu	0.47906822296566	0.53083343986032	6.80086699755659
Cu	5.63255868014557	5.00557542706274	6.73928279830916
Cu	1.75793671801733	2.75679063435941	6.73868510428021
<i>1.30 pd3_cu-h_bridge</i>			
H	6.99292274183219	5.69987070006043	11.48792207842390
Pd	4.41381004446904	-0.07956747995915	10.87625417774134
Pd	9.58564849126387	4.20713392959320	10.79562042687947
Pd	6.84615465637624	4.12764861834433	10.87708269112146
Cu	6.90482071741666	1.28652307916526	8.90760704959827
Cu	4.33873832144743	5.72968827646989	8.88417002107997
Cu	4.34569838571088	1.32018055416198	8.77433712080495
Cu	5.59472276798945	3.48396304788696	8.77678925046310
Cu	9.54013455234370	5.76448065390585	8.79158159328328
Cu	8.21069955397316	3.45955289666015	8.79307483672783
Cu	1.77261575950796	1.28451814338522	8.88313456089474
Cu	6.89667869906450	5.75342745627161	8.85553807716833
Cu	3.09539104454016	3.48387748344688	8.75940609992976
Cu	5.64060838725679	0.52793559619702	6.73737386139233
Cu	8.20695492476695	4.99553603758136	6.73341372014404
Cu	3.06224136539802	5.00032835997386	6.72938868293758
Cu	4.34692045355699	2.76110531632964	6.69481743522130
Cu	6.92791789661078	2.75776071947209	6.73876298762251
Cu	3.04871999973578	0.52090878877967	6.75224526980991
Cu	0.47856038598656	0.53097757941925	6.79735462487409
Cu	5.63724527442091	5.00506817372376	6.75314409051843
Cu	1.76492204726190	2.75329184259063	6.72947872333198
<i>1.31 pd3_cu-h_rim3</i>			
H	5.16153163510470	4.52203517525490	10.27888211803814
Pd	4.55085920657884	0.00509994577298	10.81170225387067
Pd	9.54912285291183	4.22349161740084	10.85423058592586
Pd	6.79064598148896	4.44867927748406	10.79767917849931
Cu	6.91579676168485	1.23688344651580	8.90109728066410
Cu	4.41810389622323	5.68394516074957	9.01048825999041
Cu	4.34893581768207	1.31666856695234	8.72090209703541
Cu	5.59721259145881	3.45298152543147	8.81079014002944
Cu	9.58714753883145	5.73282318943159	8.78984677520747
Cu	8.19094936667395	3.45776332579108	8.83950310058038
Cu	1.77141740358323	1.28861205140349	8.87567330469534
Cu	6.97474447455347	5.83471253046993	8.77067492351569
Cu	3.06236149811834	3.47308264425400	8.78785793679141
Cu	5.64941955910017	0.51346011594806	6.72205141507848
Cu	8.21978235268089	4.97693150054293	6.72393501248693
Cu	3.08726810897205	4.98905431574498	6.74207361529038

Cu	4.35019821250683	2.77066267157618	6.70030221741339
Cu	6.92527456839208	2.74053950464710	6.75906861726300
Cu	3.04579619735584	0.52988458326462	6.70993416034964
Cu	0.48137731447417	0.49697997742490	6.83258798057381
Cu	5.65119479435774	4.99557815652823	6.75344315104381
Cu	1.75830815037439	2.75072323118175	6.73810435472364
<i>1.32 pd3_cu-h_top</i>			
H	6.79061547271393	4.44858631906203	12.36024536144869
Pd	4.55085920657884	0.00509994577298	10.81170225387067
Pd	9.54912285291183	4.22349161740084	10.85423058592586
Pd	6.79064598148896	4.44867927748406	10.79767917849931
Cu	6.91579676168485	1.23688344651580	8.90109728066410
Cu	4.41810389622323	5.68394516074957	9.01048825999041
Cu	4.34893581768207	1.31666856695234	8.72090209703541
Cu	5.59721259145881	3.45298152543147	8.81079014002944
Cu	9.58714753883145	5.73282318943159	8.78984677520747
Cu	8.19094936667395	3.45776332579108	8.83950310058038
Cu	1.77141740358323	1.28861205140349	8.87567330469534
Cu	6.974744447455347	5.83471253046993	8.77067492351569
Cu	3.06236149811834	3.47308264425400	8.78785793679141
Cu	5.64941955910017	0.51346011594806	6.72205141507848
Cu	8.21978235268089	4.97693150054293	6.72393501248693
Cu	3.08726810897205	4.98905431574498	6.74207361529038
Cu	4.35019821250683	2.77066267157618	6.70030221741339
Cu	6.92527456839208	2.74053950464710	6.75906861726300
Cu	3.04579619735584	0.52988458326462	6.70993416034964
Cu	0.48137731447417	0.49697997742490	6.83258798057381
Cu	5.65119479435774	4.99557815652823	6.75344315104381
Cu	1.75830815037439	2.75072323118175	6.73810435472364

2 Table 2

2.1 pt3_au-h_au-site1

H	7.92686895192000	3.24666898230046	10.78923300000000
Pt	9.42878301012000	7.23284000298050	12.15411340000000
Pt	10.77293101500000	4.98765400191774	12.19264020000000
Pt	8.13839096952000	4.91159497892269	12.19709400000000
Au	7.99021299744000	1.48831502861446	10.10915880000000
Au	5.00985695628000	6.60484597371829	10.14106340000000
Au	4.99354495704000	1.52349496794095	10.27058760000000
Au	6.42709202364000	3.99253902394642	10.29096640000000
Au	11.05447299660000	6.67387196928312	10.03565680000000
Au	9.46914099768000	3.91247098894680	10.02104220000000
Au	2.06695798704000	1.48232099119088	10.16220400000000
Au	7.82284996260000	6.66105497260887	10.03434380000000
Au	3.60438101856000	4.00304803167336	10.29816840000000
Au	6.46452195192000	0.64815597278477	7.70909100000000
Au	9.42636496788000	5.75076796444051	7.71793360000000
Au	3.527066601312000	5.72108699495860	7.70566680000000
Au	5.01162098292000	3.18305299013688	7.79591020000000
Au	7.93936702620000	3.19986197247914	7.70979560000000
Au	3.53048403060000	0.64638500369620	7.69629120000000
Au	0.57711000744000	0.63007200927545	7.70795480000000
Au	6.46980499872000	5.72418900941255	7.71260360000000
Au	2.07227202984000	3.19059803478744	7.70701880000000

2.2 pt3_au-h_au-site2

H	6.49686700000000	7.43666400000000	10.92894306536176
Pt	9.49914982880591	7.22675051213433	12.20215068012793
Pt	10.81571250039946	4.96247481551679	12.17761726676784
Pt	8.19731675546845	4.95371769247413	12.19997812874828
Au	7.96853390461210	1.48529616821851	10.12958404497630
Au	5.01796118918607	6.55674544258161	10.23728955507145
Au	5.04340610177107	1.53551551802258	10.30932710079570
Au	6.46365714103171	3.99260462454378	10.31136026042359
Au	11.07490564007402	6.65623837691124	10.02810241667574
Au	9.47930210829906	3.87015149910359	10.03176303997028
Au	2.10053057844684	1.49184806946593	10.23488566360663
Au	7.95830575425758	6.60087586000885	9.98704089059116
Au	3.61791666417698	3.99592774652333	10.25005229733919
Au	6.47742989843292	0.63098399205256	7.70933760438158
Au	9.45545545011777	5.71983882786251	7.69749959903304
Au	3.566054564048672	5.71695902150337	7.71863178763280
Au	5.02238868626709	3.17060064505428	7.78339884619300
Au	7.95281098471531	3.18170315495473	7.71317903538523
Au	3.54972429366488	0.63217982985719	7.70229723137203
Au	0.58768204594698	0.61183927819014	7.72384938938139
Au	6.48178127040133	5.70904075166497	7.70579567894504
Au	2.08620951899005	3.14979019868354	7.71598095058498

2.3 pt3_au-h_au-site3

H	0.55672132295691	0.60149554902612	10.97084060070408
Pt	9.42291808760514	7.24611150290472	12.14735263374642
Pt	10.73600277632378	4.96588102316803	12.15244144893744
Pt	8.10383189302467	4.96956590117275	12.15281643348153
Au	7.89230435971462	1.47508663170285	10.26134901558929
Au	4.98091580891002	6.51540893073038	10.27259693810967
Au	4.98421833790439	1.52842752082143	10.25288075986404
Au	6.39979085501056	3.97760278065533	10.27419300746040
Au	10.99667890560705	6.62974239940977	9.99878961716767
Au	9.41292633315516	3.87914458147232	10.01449624851982
Au	2.07141958410491	1.47856523413276	10.24445645198875
Au	7.82428788096320	6.63822989705396	10.00714131336498
Au	3.56824926581162	3.97672300139078	10.25971984812452
Au	6.45222966586042	0.62300332819031	7.71220119738490
Au	9.40192558039485	5.71225952423444	7.68952436372292
Au	3.51968974866196	5.70439517354440	7.71283962470383
Au	4.97476359936468	3.15909700882933	7.75651587567063
Au	7.90975761586327	3.14649680307286	7.72238819170324
Au	3.49630416463573	0.62085215596433	7.71101325648890

Au	0.54453582966208	0.60041675311148	7.71687644027727
Au	6.43213757586604	5.70626111318177	7.72058202188338
Au	2.03611841597572	3.14565976721858	7.71286094354081
2.4	<i>pd3_au-h_au-site1</i>		
H	7.92686899999997	3.24666900000000	10.78923400000001
Pd	9.35317457549721	7.22486022047299	12.19648628170313
Pd	10.91368026375500	5.01457190827237	12.20091434320305
Pd	8.18088265659113	4.68867008860276	12.03835893298442
Au	8.00418623588063	1.48461293337653	10.15276084862842
Au	4.97605658261054	6.62151218801680	10.12234777648723
Au	4.98255428226970	1.48207411237213	10.20919556585831
Au	6.30921277792624	4.02799676214803	10.15955518996783
Au	10.99258348710422	6.69112175759021	10.07258410292335
Au	9.64370526921601	3.96436130160279	9.95225532327883
Au	2.09088224418599	1.42008290825747	10.13852141955960
Au	7.84815643854554	6.57554086883204	10.06212990099865
Au	3.57625525576434	3.99909288330639	10.16722479475237
Au	6.48049829506454	0.64607211424727	7.71229660967885
Au	9.42942087287597	5.75082158759839	7.69480855790139
Au	3.51508500937465	5.73233517357802	7.70244895582992
Au	5.00340823384819	3.15962614901205	7.71464329427045
Au	7.95914222852022	3.19923947944174	7.69314545620982
Au	3.53796603407658	0.60036290343406	7.70544210815827
Au	0.56943916843713	0.62958465507752	7.70669186369312
Au	6.46081894822334	5.71809068451731	7.70090741185899
Au	2.09117729398051	3.15060356545694	7.65254690658910
2.5	<i>pd3_au-h_au-site2</i>		
H	6.49686700000000	7.43666400000001	10.93231979908114
Pd	9.51072841979309	7.29815773540468	12.21799599220138
Pd	10.87217816011163	4.93455479568488	12.19579220387593
Pd	8.14270155069213	4.91285204456932	12.21912966402301
Au	7.98622456006619	1.47635515066806	10.13349395776683
Au	5.01103237520939	6.56680069653394	10.23744300494909
Au	5.04595458331435	1.52135190027401	10.21643284054393
Au	6.47869366985049	3.99770746549411	10.21882033828574
Au	11.03934851382260	6.62937418861858	10.07258224797993
Au	9.48530617570801	3.91972674492815	10.07953984800519
Au	2.09067984640914	1.49355976821929	10.23423472596981
Au	8.00207919858948	6.57467360194026	10.05638323141512
Au	3.60750844896539	3.99975523164968	10.16831609947683
Au	6.48843979063112	0.61852481366551	7.71588080865407
Au	9.45461672164725	5.72049033246862	7.69477190531194
Au	3.56627318091635	5.72791477240860	7.72156949373583
Au	5.02823920853776	3.16587495311142	7.73649416157067
Au	7.97105020740589	3.17904467480130	7.71904099523048
Au	3.54916639461709	0.61653540298607	7.71916051499820
Au	0.58961946989804	0.61156388407568	7.71703267214999
Au	6.49441084441449	5.72082608667656	7.72268131926723
Au	2.07924425971390	3.14486957700066	7.72357249314326
2.6	<i>pd3_au-h_au-site3</i>		
H	0.59286077281116	0.69158869318915	10.98669764606423
Pd	9.46063968119629	7.35576812222867	12.18833149322339
Pd	10.83044872372660	4.98523186464931	12.17951467182903
Pd	8.10346930822672	4.97761556533087	12.18537286740325
Au	7.92616195429400	1.55492170414047	10.26761893650210
Au	5.02145143718135	6.60955521240444	10.23084397026422
Au	5.02152920373490	1.57624913297397	10.18823556217425
Au	6.45079949395092	4.06105758941363	10.18781688719397
Au	10.99732103280793	6.67517309534211	10.05838626118476
Au	9.45866241362828	3.99640961472289	10.04814328366718
Au	2.11178347728237	1.54644240088182	10.25673950833843
Au	7.90497255843403	6.67368347210762	10.06617454683833
Au	3.60215574108331	4.05041323306850	10.17945960278012
Au	6.48691015915043	0.66599611321646	7.72372251866134
Au	9.43088652112808	5.76807184550847	7.68889416884011
Au	3.53806451872853	5.77057908922210	7.72090218911876
Au	5.00704059125488	3.21372755533167	7.71900045694833
Au	7.95237852018860	3.19793930171719	7.72765363183381
Au	3.51911347068403	0.66619738342847	7.72717470954659

Au	0.57079779890839	0.65603650872077	7.71504930344228
Au	6.47121661774106	5.77502148793086	7.72672420131725
Au	2.05727084809640	3.19404166673468	7.71827395715006
2.7	<i>pt3_cu-h_cu-site1</i>		
H	6.90960300000000	2.78169300000000	9.76853799999999
Pt	8.17177222331282	6.48461448757234	10.81500200000000
Pt	9.69472961569581	4.30278464651287	10.77917860000007
Pt	7.00000015287091	4.06416129422375	10.77530999999997
Cu	6.92496999999999	1.27518699999999	8.85785299999995
Cu	4.34610199999999	5.74025200000002	8.85887499999994
Cu	4.34833900000001	1.34293300000000	8.99550599999992
Cu	5.58699699999999	3.47807800000001	8.99636899999999
Cu	9.61346900000001	5.80684999999999	8.76174100000001
Cu	8.21507299999998	3.37893899999999	8.76425599999996
Cu	1.76537300000000	1.27386600000001	8.85670099999998
Cu	6.81304000000002	5.80670999999999	8.76131899999999
Cu	3.11623799999998	3.48066599999999	8.99536700000001
Cu	5.61696200000001	0.54041500000000	6.73146400000002
Cu	8.20621299999996	4.99227399999998	6.74018699999998
Cu	3.05609199999999	4.97635900000001	6.73198499999994
Cu	4.34473600000001	2.76426800000000	6.79621199999998
Cu	6.90524100000001	2.76524599999999	6.73367800000000
Cu	3.06848300000000	0.54406500000001	6.73159899999997
Cu	0.47665899999997	0.52823399999998	6.73563899999997
Cu	5.62819200000000	4.97640300000000	6.73268799999993
Cu	1.78240300000001	2.76740599999999	6.73243700000006
2.8	<i>pt3_cu-h_cu-site2</i>		
H	8.21101654416018	1.83269773980439	9.80457646814774
Pt	4.34856002151426	-0.05472207737063	10.75113009650318
Pt	9.56347264701704	4.34253958248187	10.82442094343378
Pt	6.86504909057721	4.34219229758475	10.82583288492082
Cu	6.88971816353630	1.23627383391578	8.95024146196566
Cu	4.34546126199309	5.67722355024766	8.95196211668940
Cu	4.34579769341742	1.34335280380775	8.73166807793791
Cu	5.59952760029207	3.48265954242709	8.83067481608353
Cu	9.54242966878417	5.76862400088791	8.75151966363098
Cu	8.21123577243579	3.39394300124100	8.85755411380343
Cu	1.80053797722475	1.23577332762969	8.94855548698675
Cu	6.88026760034643	5.76883804560965	8.75333058592586
Cu	3.09177775407291	3.48177014033621	8.82782937320223
Cu	5.650757432126281	0.53072039809043	6.72212974502680
Cu	8.20966883582570	4.96522487936227	6.72581970940699
Cu	3.06246542253478	4.99382439912306	6.74197104159856
Cu	4.34454644291093	2.77103992347773	6.70154274904317
Cu	6.91998000973696	2.75165632857350	6.74403930310101
Cu	3.03822839190495	0.53086598722951	6.72268894855601
Cu	0.47910754505635	0.50959278983397	6.80645248066123
Cu	5.62657730269912	4.99423151876869	6.74346075187885
Cu	1.76859214973560	2.75148710472180	6.74316064865515
2.9	<i>pt3_cu-h_cu-site3</i>		
H	0.48069307981122	0.54118507173628	9.83722902232320
Pt	8.21335967363192	6.58462125884163	10.76759853454937
Pt	9.55754710960479	4.26656827864124	10.78039892456553
Pt	6.86790231526599	4.26685360293594	10.78145455345381
Cu	6.90378518688569	1.29009844954688	8.99698322820863
Cu	4.34532431153373	5.70506992190968	9.04204962335866
Cu	4.34529580181078	1.33892838120271	8.75707886758863
Cu	5.58924274994099	3.48168718673833	8.79263783578353
Cu	9.54385086117089	5.77572575546639	8.75551553666229
Cu	8.21089295656826	3.46241873458005	8.78223632687441
Cu	1.78597663347892	1.28968401250014	8.99436319455011
Cu	6.87767578221662	5.77616877457722	8.75744695033693
Cu	3.10129168879215	3.48146678187285	8.78988422988805
Cu	5.65012170119059	0.53560844527445	6.72970165519300
Cu	8.20894204505306	4.99047575714142	6.70365967007181
Cu	3.07052938761916	5.00160121662614	6.74174910576748
Cu	4.34430338664239	2.76633891818546	6.69296037672905
Cu	6.92637954663512	2.74156338450251	6.74733863538335
Cu	3.03761505630122	0.53566159098304	6.73017380501446

Cu	0.47831375585260	0.52334269021737	6.80456049566656
Cu	5.61734835760512	5.00188848311423	6.74340780148426
Cu	1.76166355444911	2.74150138105390	6.74614084111999
<i>2.10 pd3_cu-h_cu-site1</i>			
H	6.90960300000000	2.78169300000000	9.52658356345994
Pd	8.21620496840482	6.58550497087918	10.82319223597793
Pd	9.59047728809736	4.20687720452577	10.82426992205589
Pd	6.84174297621973	4.20553586833233	10.82465432719258
Cu	6.91361098220897	1.28173141234640	8.89734377913174
Cu	4.34607824580669	5.72836957849940	8.89768691171086
Cu	4.34587566048038	1.31556759440731	8.77341163455913
Cu	5.60112425376055	3.48822619764721	8.77722840574186
Cu	9.54253548096757	5.76397209521768	8.81134450548304
Cu	8.21299443137915	3.45927415741260	8.81438693958250
Cu	1.77762453293883	1.28063658047884	8.89590213150742
Cu	6.88171635780982	5.76442723593863	8.81344526339235
Cu	3.09173318653008	3.48740627250601	8.77446049103726
Cu	5.64052818489001	0.52880317100014	6.73552373170201
Cu	8.20936217421047	4.99372183300449	6.73250272520257
Cu	3.05810920268361	5.00149067746129	6.73575512979583
Cu	4.34500250400048	2.76285266775907	6.69826163547518
Cu	6.9270333293750	2.75669338102469	6.73738747028649
Cu	3.04810793398826	0.52887591697075	6.73590322795272
Cu	0.47892488848570	0.53057389757936	6.80200188004687
Cu	5.63062377475880	5.00175926926601	6.73730095868185
Cu	1.76203135213493	2.75656290534914	6.73619493238634
<i>2.11 pd3_cu-h_cu-site2</i>			
H	8.23244400057598	1.89362164802006	9.80514226825324
Pd	8.21858955236393	6.67521408636087	10.79994285547094
Pd	9.67206465859962	4.35792772146675	10.84419656776898
Pd	6.87805542428080	4.30192622753477	10.85587409822542
Cu	6.92134956747021	1.25006164628969	8.93019116975923
Cu	4.35182784020928	5.68425636918289	8.92162713620026
Cu	4.36384620616512	1.32512073486137	8.72431791246084
Cu	5.62640576908606	3.49124037821657	8.80709800262907
Cu	9.52992307660920	5.77368131028497	8.77682753197370
Cu	8.24915905757239	3.44102305193757	8.88193064813510
Cu	1.80707660706835	1.23634063666281	8.92560810264859
Cu	6.91372842207486	5.75571136015462	8.78937627005855
Cu	3.10596683670337	3.48529602810103	8.79104616155634
Cu	5.66321259464061	0.53236479267199	6.72497630415325
Cu	8.22046062886552	4.96717958603338	6.73250231251423
Cu	3.06861034043650	4.99713290096192	6.74324577774570
Cu	4.35828122462551	2.76681212988269	6.70135815503454
Cu	6.93790941853585	2.75368856951404	6.74850405065021
Cu	3.04825230505426	0.52671090087532	6.72995274121319
Cu	0.48976959674699	0.51071703941074	6.79006030233571
Cu	5.63930825535244	4.99610341275227	6.74852840146242
Cu	1.77698069416096	2.74990865025811	6.74276736491625
<i>2.12 pd3_cu-h_cu-site3</i>			
H	0.47735314322842	0.51398800428854	9.81811060214128
Pd	8.23434700517275	6.56192449065751	10.81900320917354
Pd	9.60937302330638	4.18141091192959	10.81250838820416
Pd	6.86075699683913	4.17566690066272	10.82169060020055
Cu	6.90340025752492	1.26515597031148	8.96539430064742
Cu	4.34156823621472	5.70468393455634	8.95982277028470
Cu	4.34359963585550	1.30083075477606	8.76772231364740
Cu	5.59747546819557	3.46967624761500	8.77513158117014
Cu	9.51838543973057	5.72908444508830	8.79320813300645
Cu	8.21556405942012	3.46362244499943	8.79905922486421
Cu	1.77907658177511	1.26307886937591	8.95704504063088
Cu	6.90139554634135	5.73339053432090	8.80817263217291
Cu	3.09655833521523	3.46562803527625	8.75699562808531
Cu	5.64931657333889	0.52091407970688	6.74401689497281
Cu	8.20651808804394	4.98247774477416	6.71265745177742
Cu	3.06573465942264	4.99737242070863	6.74042168622085
Cu	4.34629250887348	2.75037931969527	6.69423372220198
Cu	6.92687962539553	2.73565763996110	6.74716477827945
Cu	3.03564520790736	0.52027042657999	6.74610009016123

Cu	0.47612044673253	0.52141204308473	6.77464076536955
Cu	5.62039425413747	4.99824585337146	6.74831852146643
Cu	1.75921777035577	2.73498004691461	6.74098094459707
<i>2.13 au-h_fcc</i>			
H	7.93753863696696	4.88009762408353	10.89072059172093
Au	7.92897103127159	1.45840465181443	10.10370255012754
Au	4.97232715870823	6.58518692867875	10.10232938808277
Au	4.96999002290453	1.47386473688451	10.11449128364231
Au	6.40474760038492	3.99490319725091	10.20363418573862
Au	10.89239555595460	6.58803856511759	10.10215084491611
Au	9.46710065167765	3.99356680220757	10.20661943920129
Au	2.03354987431397	1.47110906163458	10.11469524564773
Au	7.93597399665616	6.64499428163085	10.20630157754976
Au	3.50270269908308	4.01416006230039	10.11960442093481
Au	6.44994266409768	0.60983070367858	7.69980096644152
Au	9.39743904041957	5.71765189134199	7.70989908090743
Au	3.49978346376602	5.71959675481183	7.70047902216173
Au	4.99388218384497	3.17982081331254	7.71320918181510
Au	7.92893659769024	3.17419395007630	7.71018438548987
Au	3.50084566643625	0.59223505194375	7.71142193675808
Au	0.54932693467755	0.60893850785257	7.70018028109850
Au	6.46033142150524	5.71928665042616	7.70972807079345
Au	2.00950924676762	3.17358343329890	7.71239659170654
<i>2.14 cu-h_fcc</i>			
H	6.92830989575482	4.25131402538901	9.76144759579013
Cu	6.92678272082930	1.26253572344457	8.79063260308194
Cu	4.33789941243480	5.74685298134243	8.79074819922853
Cu	4.34902431598716	1.27674371851755	8.79760593391730
Cu	5.63797566473496	3.50773391503827	8.85133763745348
Cu	9.51578698221859	5.74671850183961	8.79088606986977
Cu	8.21633425792583	3.50744601396554	8.85104328409208
Cu	1.77419876354932	1.27679390612997	8.79745086639407
Cu	6.92696812957522	5.74018763993565	8.85163890372813
Cu	3.06161738374017	3.50718452853449	8.79748197998883
Cu	5.63163350468310	0.53371260730700	6.73210780608161
Cu	8.21339950913428	4.99506945016081	6.72654925326476
Cu	3.05867668946604	4.99014526567201	6.73209042744251
Cu	4.36395565562224	2.77269270394003	6.74673623577668
Cu	6.92393674887390	2.76176785221795	6.72637610081816
Cu	3.05898923111204	0.51195125313286	6.74661778504117
Cu	0.48593938493244	0.53375533996270	6.73192729752789
Cu	5.63446474005356	4.99522375495322	6.72661651326358
Cu	1.75403208618727	2.77251711106709	6.74645735215333

3 Table 3

<i>3.1 pt3_au-h_rim1_to_au-site4_TS</i>			
H	5.34437546832962	5.16711909141020	11.16320288129863
Pt	9.41360324213599	7.27168887699785	12.19545265390974
Pt	10.70496621501722	5.00149087814842	12.16769008066538
Pt	8.04945121914353	5.01887431749887	12.19397529868577
Au	7.95461381109620	1.49273877974418	10.13723590303407
Au	5.00687318517393	6.62482637729562	10.11009027916745
Au	5.00305911461245	1.56111655013834	10.30509683628755
Au	6.40243999855377	4.01409421582023	10.27845043264040
Au	11.03425516037916	6.68530332334069	10.04056395076515
Au	9.42454812822440	3.89402091946800	10.03348477459083
Au	2.05178304435495	1.49586329843314	10.16065314194418
Au	7.84077486996199	6.68648865177015	10.01938155059429
Au	3.55103707731208	4.01088359951872	10.28500941867512
Au	6.45757368838779	0.63721067068211	7.70752154801595
Au	9.42613941725760	5.73865420608714	7.71829592510593
Au	3.53000743782526	5.72040564376673	7.71182354579158
Au	4.99422836870605	3.18859895305718	7.79706893499708
Au	7.93255471269556	3.18822125986929	7.71147693888639
Au	3.53168157299012	0.64549611686846	7.70677492240065
Au	0.57326903916229	0.63559576650368	7.70829280931991
Au	6.47339109549448	5.71749798778346	7.70786638627180
Au	2.06269031523368	3.18712355074374	7.69734651323988
<i>3.2 pd3_au-h_rim2_to_au-site4_TS</i>			
H	5.36969115905337	5.22432128631367	11.14510526802066
Pd	9.50448156866995	7.44277709023990	12.21846463340161
Pd	10.87697235862197	5.08989500885427	12.22026337893013
Pd	8.14130534163021	5.05483984601934	12.18382338220047
Au	7.97389009818123	1.54816717216480	10.12830001425665
Au	5.00749161216614	6.68882073248146	10.12141079349487
Au	4.99327245584172	1.57818051136662	10.16281286756222
Au	6.38589766226578	4.06325450153732	10.24814138562675
Au	11.00809056388680	6.72413766682925	10.06939879638968
Au	9.47292739714596	3.99338227595735	10.10393726564132
Au	2.04505447208234	1.53487750515158	10.13633432368660
Au	7.89190380364103	6.73251008049454	10.09456205671127
Au	3.53821154792713	4.07836674353061	10.16746951098018
Au	6.46986294104307	0.67480096941906	7.70231755728946
Au	9.42341186011058	5.77493042607887	7.72814249245806
Au	3.52379835438439	5.77332015714437	7.70515978361925
Au	5.01378213550321	3.23619208362911	7.75280569137442
Au	7.94353964660316	3.24041003521706	7.73671299876601
Au	3.52625175398313	0.66301274040804	7.70030629241879
Au	0.571733668884815	0.66772602908977	7.70062295879909
Au	6.48350075467458	5.76868868348761	7.73057411653400
Au	2.04590437122134	3.22290488900351	7.70109360226697
<i>3.3 pt3_cu-h_rim1_to_cu-site4_TS</i>			
H	4.16394985760105	4.26354891380850	9.92182373267360
Pt	8.33541865970082	6.58874586575845	10.78970278433620
Pt	9.54714368212223	4.21483981638087	10.80291112501886
Pt	6.87372582267307	4.32254439564461	10.81994217772437
Cu	6.90387835618626	1.26931883688910	8.93225296903735
Cu	4.38053055697777	5.73286259766750	8.90572005967560
Cu	4.35072281161130	1.33679947793231	8.77537062040927
Cu	5.60406174712917	3.48258170445042	8.83109542024058
Cu	9.59871626175219	5.75778340395085	8.76722756724980
Cu	8.21457694227142	3.42419518396112	8.79147244290185
Cu	1.78420778335637	1.29325345907710	8.90239278853704
Cu	6.90216303714231	5.81266488519589	8.78884338121743
Cu	3.09457284085480	3.48217766991867	8.78753840396994
Cu	5.64459114944624	0.52560147440996	6.72842308038581
Cu	8.21505234745721	4.98982484167140	6.72705509575499
Cu	3.07799639292661	4.99733190779465	6.72895314700686
Cu	4.35589244338591	2.77130654129402	6.71094591084101
Cu	6.92728086898851	2.75229374920667	6.74724224673392

Cu	3.05185409618429	0.53173165359316	6.72657203437956
Cu	0.48000171178160	0.53005779804153	6.82065830494908
Cu	5.64376139084525	4.99871029925302	6.74839171861243
Cu	1.76765706850612	2.75464291690456	6.72598191060796
3.4	<i>pd3_cu-h_rim3_to_cu-site4_TS</i>		
H	4.02856359526003	4.27405085461717	9.97535289409820
Pd	4.55085915385425	0.00509991731335	10.81170220050642
Pd	9.54912281667029	4.22349158904401	10.85423051150644
Pd	6.79064594126996	4.44867926883274	10.79767913978149
Cu	6.91579679726005	1.23688345882808	8.90109717030737
Cu	4.41810388639651	5.68394514512876	9.01048830090188
Cu	4.34893582327201	1.31666859833634	8.72090215632767
Cu	5.59721260492914	3.45298150287950	8.81079018437259
Cu	9.58714750235074	5.73282315755783	8.78984682896873
Cu	8.19094937950784	3.45776335320295	8.83950309795704
Cu	1.77141742547200	1.28861202363820	8.87567328041735
Cu	6.97474443706089	5.83471251349483	8.77067485294204
Cu	3.06236151085685	3.47308265377725	8.78785802724126
Cu	5.64941955278374	0.51346014106363	6.72205134038659
Cu	8.21978236714264	4.97693149987387	6.72393506220995
Cu	3.08726814225648	4.98905433096821	6.74207371468705
Cu	4.35019820041204	2.77066266976805	6.70030229673295
Cu	6.92527459804880	2.74053949647786	6.75906851680400
Cu	3.04579623160323	0.52988460894358	6.70993424301971
Cu	0.48137733508262	0.49697997296575	6.83258791002243
Cu	5.65119480445754	4.99557815205091	6.75344322413988
Cu	1.75830814521479	2.75072326373404	6.73810428159202

4 Table S2

4.1	<i>pt3_au-h_bridge_to_rim1_TS</i>		
H	7.52755765741458	6.05360638018980	13.28190149297016
Pt	9.33116447023131	7.32375549678283	12.23780353838006
Pt	10.67087665698952	5.02847836854907	12.07971362588668
Pt	8.01985785010922	4.96757845902434	12.24183140018864
Au	7.94394477861775	1.47324388832260	10.15521791175982
Au	4.96053955181114	6.58062590285138	10.14534089048024
Au	4.98899717368342	1.55303796274548	10.29006520685007
Au	6.39988246351923	3.99447811595426	10.28102928976831
Au	10.97266864794397	6.72201889964086	10.02250914448045
Au	9.36989763925677	3.87344968547201	10.02652832406220
Au	2.02913113518679	1.46980127281678	10.14473069752850
Au	7.81619827576423	6.63899698784994	10.04264505117402
Au	3.55577468723637	4.00173823231181	10.30405777496604
Au	6.44745490303165	0.63672927914943	7.69804157347373
Au	9.41117519783774	5.72064145500378	7.71656434956205
Au	3.50242355277403	5.70253210435049	7.71347527707013
Au	4.97499128688546	3.17718905788000	7.78651814190337
Au	7.91367004551105	3.16919268744895	7.70296429229461
Au	3.52676735669867	0.62361126701882	7.72115686587453
Au	0.55449295572481	0.60635325944310	7.72298815935751
Au	6.45352580306365	5.70582504462040	7.71842015627621
Au	2.05387281147417	3.16884180901933	7.70813898487634
4.2	<i>pt3_au-h_bridge_to_three-fold_TS</i>		
H	9.19448822296712	5.86500664220298	13.26675889116281
Pt	9.33116447023130	7.32375549678281	12.23780353838006
Pt	10.67087665698952	5.02847836854906	12.07971362588668
Pt	8.01985785010922	4.96757845902434	12.24183140018864
Au	7.94394477861774	1.47324388832260	10.15521791175982
Au	4.96053955181114	6.58062590285137	10.14534089048024
Au	4.98899717368342	1.55303796274548	10.29006520685007
Au	6.39988246351923	3.99447811595426	10.28102928976831
Au	10.97266864794396	6.72201889964086	10.02250914448045
Au	9.36989763925676	3.87344968547200	10.02652832406220
Au	2.02913113518679	1.46980127281678	10.14473069752850
Au	7.81619827576423	6.63899698784994	10.04264505117402
Au	3.55577468723637	4.00173823231181	10.30405777496604
Au	6.44745490303165	0.63672927914943	7.69804157347373
Au	9.41117519783774	5.72064145500377	7.71656434956205
Au	3.50242355277403	5.70253210435048	7.71347527707013
Au	4.97499128688546	3.17718905788000	7.78651814190337
Au	7.91367004551105	3.16919268744895	7.70296429229461
Au	3.52676735669867	0.62361126701882	7.72115686587453
Au	0.55449295572481	0.60635325944310	7.72298815935751
Au	6.45352580306365	5.70582504462040	7.71842015627621
Au	2.05387281147417	3.16884180901932	7.70813898487634
4.3	<i>pd3_au-h_bridge_to_rim2_TS</i>		
H	7.06146662541887	6.19285016364175	11.87184874723977
Pd	9.50448156866995	7.44277709023990	12.21846463340161
Pd	10.87697235862197	5.08989500885427	12.22026337893013
Pd	8.14130534163021	5.05483984601934	12.18382338220047
Au	7.97389009818123	1.54816717216480	10.12830001425665
Au	5.00749161216614	6.68882073248146	10.12141079349487
Au	4.99327245584172	1.57818051136662	10.16281286756222
Au	6.38589766226578	4.06325450153732	10.24814138562675
Au	11.00809056388680	6.72413766682925	10.06939879638968
Au	9.47292739714596	3.99338227595735	10.10393726564132
Au	2.04505447208234	1.53487750515158	10.13633432368660
Au	7.89190380364103	6.73251008049454	10.09456205671127
Au	3.53821154792713	4.07836674353061	10.16746951098018
Au	6.46986294104307	0.67480096941906	7.70231755728946
Au	9.42341186011058	5.77493042607887	7.72814249245806
Au	3.52379835438439	5.77332015714437	7.70515978361925
Au	5.01378213550321	3.23619208362911	7.75280569137442
Au	7.94353964660316	3.24041003521706	7.73671299876601
Au	3.52625175398313	0.66301274040804	7.70030629241879

Au	0.57173366884815	0.66772602908977	7.70062295879909
Au	6.48350075467458	5.76868868348761	7.73057411653400
Au	2.04590437122134	3.22290488900351	7.70109360226697
4.4	<i>pd3_au-h_bridge_to_three-fold_TS</i>		
H	8.65693534911768	6.16343446544463	13.00891484375449
Pd	9.41591568767324	7.36517715936847	12.20920877967768
Pd	10.81885151345631	4.93595781030256	12.21479588357137
Pd	8.01466704033415	4.93534757074826	12.21383168143980
Au	7.93455644012839	1.46814684225615	10.13732023387954
Au	4.97952180974379	6.57911722212550	10.13807090437838
Au	4.98548636263441	1.53754673718682	10.18202577326441
Au	6.41158003709351	3.99958864693591	10.19078526898063
Au	10.97230535406553	6.63639808840195	10.09038946517592
Au	9.41252153203213	3.92324001596626	10.10075054908244
Au	2.02430552634756	1.46670743874688	10.13335048860607
Au	7.84541106281624	6.64071498354453	10.09420402715418
Au	3.55948744687801	3.99625199431652	10.19274985731730
Au	6.44089462480556	0.61112792246201	7.71958882036022
Au	9.40167524168280	5.72387462300662	7.72131574807528
Au	3.49289778714271	5.71373243009534	7.72170076835768
Au	4.97609731775696	3.16956257366203	7.70332794846147
Au	7.92385158204396	3.17827341294221	7.72340435472018
Au	3.51175067138107	0.61362139625967	7.71992974117971
Au	0.54676944691632	0.60935340112994	7.71577021004244
Au	6.45766083144425	5.71514969761540	7.72260720903597
Au	2.02795617817933	3.17979772009862	7.72266809528243
4.5	<i>pt3_cu-h_bridge_to_rim1_TS</i>		
H	6.18217598574459	5.45757453187938	11.36863104883135
Pt	8.29557830748673	6.57580048373787	10.84628382208669
Pt	9.56250512034488	4.21659017754806	10.74303048988040
Pt	6.88528863683717	4.13393351412291	10.847244444647101
Cu	6.90182642259576	1.28401698850575	8.94856535439054
Cu	4.33924875889324	5.72309827531809	8.90932469326962
Cu	4.34718033172665	1.32386612118883	8.80337475373503
Cu	5.59208151025800	3.47768740906494	8.80588646913029
Cu	9.56154359837137	5.77459887814781	8.74970000242607
Cu	8.20903374512083	3.43060479735044	8.75218561859436
Cu	1.77541479936690	1.28443143034383	8.90754135667762
Cu	6.88277159195107	5.76019856958321	8.82439716079756
Cu	3.11432120655786	3.47155127888665	8.76934074047031
Cu	5.63918017128215	0.53323301783391	6.73399270235077
Cu	8.20717192983149	4.99250221266055	6.71561375895596
Cu	3.06594028439905	4.99501581275239	6.72189894005403
Cu	4.35075165321193	2.75700238271427	6.69902934094839
Cu	6.92066083031581	2.75118661785113	6.73525554771721
Cu	3.04972567483085	0.52438897179174	6.75256822053072
Cu	0.47453311199336	0.53060092976319	6.82849279408148
Cu	5.63367001465917	4.99917336046385	6.75346886091612
Cu	1.76962227145958	2.74962874102316	6.72259812403734
4.6	<i>pt3_cu-h_bridge_to_three-fold_TS</i>		
H	8.25364831314981	4.41287262582883	11.76926199999996
Pt	8.29557800000001	6.57579999999999	10.84628399999996
Pt	9.56250500000002	4.21659000000002	10.74303100000000
Pt	6.88528900000001	4.13393400000001	10.84724399999993
Cu	6.90182599999998	1.28401700000000	8.94856500000004
Cu	4.33924900000001	5.72309800000001	8.90932499999997
Cu	4.34717999999998	1.32386599999999	8.80337399999999
Cu	5.59208200000001	3.47768700000002	8.80588599999997
Cu	9.56154300000001	5.77459900000002	8.74970000000006
Cu	8.20903399999997	3.43060499999998	8.75218600000007
Cu	1.77541500000000	1.28443100000000	8.90754099999996
Cu	6.88277100000000	5.76019899999998	8.82439700000003
Cu	3.11432100000002	3.47155100000000	8.76934099999994
Cu	5.63917999999997	0.53323300000001	6.73399300000003
Cu	8.20717200000001	4.99250200000000	6.71561399999994
Cu	3.06594000000001	4.99501599999998	6.72189900000000
Cu	4.35075199999998	2.75700199999999	6.69902899999995
Cu	6.92066099999999	2.75118700000001	6.73525599999997
Cu	3.04972599999998	0.52438900000002	6.75256799999993

Cu	0.47453300000001	0.53060100000000	6.82849299999994
Cu	5.63367000000002	4.99917300000002	6.75346900000003
Cu	1.76962199999998	2.74962899999998	6.72259800000002
4.7	<i>pd3_cu-h_bridge_to_rim3_TS</i>		
H	6.02542217541168	5.48345076526584	10.40161564777503
Pd	8.27901867905535	6.61517025714059	10.87625417774139
Pd	9.58564849123412	4.20713392960822	10.79562042687943
Pd	6.84615465635496	4.12764861835905	10.87708269112152
Cu	6.90482071739524	1.28652307916985	8.90760704959829
Cu	4.33873832143395	5.72968827649031	8.88417002108000
Cu	4.34569838569740	1.32018055416669	8.77433712080494
Cu	5.59472276797206	3.48396304789939	8.77678925046311
Cu	9.54013455231404	5.76448065392639	8.79158159328335
Cu	8.21069955394768	3.45955289667249	8.79307483672783
Cu	1.77261575950247	1.28451814338982	8.88313456089477
Cu	6.89667869904308	5.75342745629212	8.85553807716839
Cu	3.09539104453054	3.48387748345930	8.75940609992977
Cu	5.64060838723926	0.52793559619892	6.73737386139232
Cu	8.20695492474146	4.99553603759918	6.73341372014400
Cu	3.06224136538850	5.00032835999169	6.72938868293763
Cu	4.34692045354351	2.76110531633950	6.69481743522132
Cu	6.92791789658927	2.75776071948194	6.73876298762256
Cu	3.04871999972632	0.52090878878153	6.75224526980997
Cu	0.47856038598506	0.53097757942113	6.79735462487412
Cu	5.63724527440338	5.00506817374162	6.75314409051836
Cu	1.76492204725641	2.75329184260046	6.72947872333198
4.8	<i>pd3_cu-h_bridge_to_three-fold_TS</i>		
H	7.55302960103290	5.37695736083085	11.80097903771836
Pd	8.27901867905535	6.61517025714059	10.87625417774139
Pd	9.58564849123412	4.20713392960822	10.79562042687943
Pd	6.84615465635496	4.12764861835905	10.87708269112152
Cu	6.90482071739524	1.28652307916985	8.90760704959829
Cu	4.33873832143395	5.72968827649031	8.88417002108000
Cu	4.34569838569740	1.32018055416669	8.77433712080494
Cu	5.59472276797206	3.48396304789939	8.77678925046311
Cu	9.54013455231404	5.76448065392639	8.79158159328335
Cu	8.21069955394768	3.45955289667249	8.79307483672783
Cu	1.77261575950247	1.28451814338982	8.88313456089477
Cu	6.89667869904308	5.75342745629212	8.85553807716839
Cu	3.09539104453054	3.48387748345930	8.75940609992977
Cu	5.64060838723926	0.52793559619892	6.73737386139232
Cu	8.20695492474146	4.99553603759918	6.73341372014400
Cu	3.06224136538850	5.00032835999169	6.72938868293763
Cu	4.34692045354351	2.76110531633950	6.69481743522132
Cu	6.92791789658927	2.75776071948194	6.73876298762256
Cu	3.04871999972632	0.52090878878153	6.75224526980997
Cu	0.47856038598506	0.53097757942113	6.79735462487412
Cu	5.63724527440338	5.00506817374162	6.75314409051836
Cu	1.76492204725641	2.75329184260046	6.72947872333198

5 Table S3

5.1 pt3_au-h_au-site4

H	6.47696779724549	2.33427394922007	10.96873379952747
Pt	9.46463252954208	7.22977309654068	12.19665696700031
Pt	10.78774946429336	4.96052706520551	12.16509970257576
Pt	8.16100822767697	4.97839898324627	12.19988101151995
Au	7.98490781222947	1.45531113162704	10.20003760766518
Au	4.99086143682080	6.61131649423518	10.14740081198375
Au	4.89984638469307	1.53378863935074	10.32835056675472
Au	6.38123536841762	4.09367137249647	10.33765541808630
Au	11.01331582529917	6.65929083555474	10.01846030478219
Au	9.42174184527189	3.90018111313766	10.02680021025384
Au	2.02353284685017	1.47516043064297	10.14418997040920
Au	7.82457397726171	6.66640736940082	10.04682492071146
Au	3.55518367233063	4.01801093149266	10.22276730950753
Au	6.44619582172971	0.63594535645323	7.71181662182681
Au	9.40171029679856	5.73356262455426	7.71346306924855
Au	3.50830116050837	5.71594777190284	7.69742023319309
Au	4.98731131396405	3.17569666302495	7.77067043487431
Au	7.91641099768668	3.17410543842314	7.71713211422598
Au	3.52502778830060	0.63798184294280	7.70958674127813
Au	0.54360560919816	0.61959177117877	7.71939725326142
Au	6.45466729143366	5.70646883940578	7.71509524833687
Au	2.04165528483476	3.17572669250253	7.69960057796368

5.2 pd3_au-h_au-site4

H	6.50226271702453	2.36081688964980	10.91327318415810
Pd	9.50554018460631	7.30099758336789	12.22275718853778
Pd	10.87728393162659	4.94842438583495	12.18393066193066
Pd	8.15652644755399	4.95759295547510	12.22049596067385
Au	8.03081612304454	1.46861707829385	10.20765159596363
Au	5.02443687469151	6.63437351512085	10.13248189374472
Au	4.95041816216398	1.53010519585567	10.24478109864730
Au	6.43737028641141	4.11551338148708	10.25250177547121
Au	11.00847911578088	6.65417789887833	10.06017821599456
Au	9.46068846734808	3.96919296858081	10.06079703696095
Au	2.05773633176504	1.49566607051260	10.13071902458644
Au	7.89619922660783	6.66496900799095	10.09179072509278
Au	3.58423712848160	4.03557064328243	10.15068471005144
Au	6.47342166355477	0.64871271708704	7.71814362577106
Au	9.42779161418474	5.75868184573337	7.71307801729682
Au	3.53031344448197	5.75055475934320	7.70066893113299
Au	5.01105893900933	3.19586785534896	7.73098397721961
Au	7.94856328886011	3.20266636133763	7.72363947245094
Au	3.54264900482523	0.64967801287567	7.71620846740803
Au	0.56483143109973	0.64835983664318	7.71275467533433
Au	6.48418002898996	5.73810651598751	7.71983683176376
Au	2.05537470994455	3.19899467445975	7.69849582988851

5.3 pt3_cu-h_cu-site4

H	5.61820312857753	2.07361682070179	9.92798200635033
Pt	4.39368249295646	-0.23204659393240	10.82554295467722
Pt	9.63740383462524	4.16548971198565	10.75873982629814
Pt	6.95115129385782	4.17179655618798	10.80876014532105
Cu	6.90168662988587	1.29432412318039	8.98219341418470
Cu	4.32869425022247	5.73257355167627	8.90643844809336
Cu	4.34014128648597	1.32567910844651	8.85839973268198
Cu	5.57934013667801	3.48890468378988	8.83190855846463
Cu	9.55988448712181	5.75838030074934	8.76733001336149
Cu	8.23240860447505	3.44611727976894	8.75436090252558
Cu	1.77106431918587	1.29030901394018	8.91102461267459
Cu	6.84912935421762	5.77560053893360	8.80989829813571
Cu	3.10013021008972	3.48023120166489	8.72206554482797
Cu	5.63352370529761	0.53459549685952	6.73826257804238
Cu	8.19838178458298	5.00179234462647	6.71714448252938
Cu	3.05803974950885	5.00656728720224	6.71501083269880
Cu	4.35162839581107	2.75516670496597	6.69439239100701
Cu	6.92010876300712	2.76057934773105	6.73216468465568
Cu	3.05263390235363	0.53908338011944	6.75776518328157

Cu	0.46080893402378	0.54243284714956	6.84105206045377
Cu	5.62262009861964	4.99418666366184	6.75247935729995
Cu	1.75950809460685	2.75198593348018	6.71205366613993
5.4 <i>pd3_cu-h_cu-site4</i>			
H	5.59087263768511	2.05236507852794	9.85573388333886
Pd	8.23972575114291	6.54798399037638	10.84598091875206
Pd	9.62525584392553	4.18583456071291	10.82269691627151
Pd	6.88601918637351	4.19533884449150	10.84413809717222
Cu	6.90971833270471	1.28791869023502	8.95317426833917
Cu	4.34255089989655	5.73641129397388	8.87937139429053
Cu	4.34086380117994	1.32200085070227	8.81003874456970
Cu	5.59362923631591	3.49311634606080	8.80882331794037
Cu	9.53719314121267	5.74988111333511	8.80571800788311
Cu	8.22580986233688	3.47501548060249	8.80516480403971
Cu	1.77180016190841	1.28278346852404	8.87901358479729
Cu	6.88263799634756	5.76430084479629	8.81464374430235
Cu	3.07766946156335	3.49756708418435	8.74844757914595
Cu	5.64076149881944	0.52772272568935	6.73585704413021
Cu	8.20708329377145	4.99816103333937	6.72937033955719
Cu	3.05930483921992	5.00758107738673	6.72829673765964
Cu	4.34563410152382	2.76345818101739	6.69959312005415
Cu	6.93083763459324	2.76092982533289	6.73624593228146
Cu	3.05713568448693	0.53445419957871	6.74706215656279
Cu	0.46560051800345	0.54095882883143	6.81284260964152
Cu	5.63163144709436	4.99378890515969	6.74699332454085
Cu	1.75980568472789	2.75563216200141	6.72800767014345
5.5 <i>pt3_au_6layers</i>			
Pt	10.72892865185230	4.96802993184437	19.42953356674469
Pt	8.10582955000815	4.96862680802939	19.42893458742403
Pt	9.41652940128048	7.24109725767745	19.43070948718485
Au	7.93474271310993	1.45698593495791	17.399973692255660
Au	11.01594641035518	6.65039501204252	17.28618277411758
Au	4.97863052002246	6.57500160129296	17.39993546630619
Au	6.40783256044492	3.98654573502475	17.52796165716694
Au	9.41328701559626	3.86268361798013	17.29098178349671
Au	4.98355483023880	1.52916047248000	17.52820405151797
Au	2.02038355996970	1.45534776237376	17.39751181090123
Au	7.80131622032696	6.65408377294525	17.29261006609013
Au	3.56646442274680	3.98525027848703	17.52769344169358
Au	6.43711502109739	0.61422600782165	14.95626067624327
Au	9.40060030351134	5.71602174256630	14.96815408221196
Au	3.49894052720991	5.70239754794779	14.95588633121453
Au	4.97662659298263	3.16455979004953	15.01642579665604
Au	7.91237862535998	3.16635473791745	14.95923002447126
Au	3.50943537025128	0.61446357693746	14.95629558946592
Au	0.54394078554667	0.60329431384419	14.96060286486797
Au	6.44766987273362	5.70554505011756	14.96027363505304
Au	2.03595296131799	3.16355456133937	14.95611998200569
Au	10.87900700000000	4.86678000000002	12.55009900000005
Au	4.97582700000000	4.86676900000000	12.55009900000005
Au	6.45157400000000	2.31063900000000	12.55009900000005
Au	9.40320800000002	2.31061899999998	12.55009900000005
Au	7.92737400000002	4.86679999999998	12.55009900000005
Au	3.50002699999999	2.31060800000002	12.55009900000005
Au	12.35480900000002	7.42294100000000	12.55009900000005
Au	9.40317300000000	7.42296000000001	12.55009900000005
Au	6.45162700000002	7.42292999999998	12.55009900000005
Au	7.92736799999998	1.45858900000001	10.14010000000005
Au	10.87896700000004	6.57091000000002	10.14010000000005
Au	4.97578600000004	6.57090000000001	10.14010000000005
Au	6.45162100000004	4.01471900000002	10.14010000000005
Au	9.40316799999999	4.01474999999999	10.14010000000005
Au	4.97582099999999	1.45855899999999	10.14010000000005
Au	2.02418599999998	1.45857800000000	10.14010000000005
Au	7.92742099999999	6.57088000000000	10.14010000000005
Au	3.49998699999999	4.01473899999998	10.14010000000005
Au	6.45161499999997	0.60650799999999	7.73010000000004
Au	9.40321400000003	5.71883000000001	7.73010000000004
Au	3.50003300000003	5.71881899999999	7.73010000000004

Au	4.975779999999997	3.162688999999999	7.730100000000004
Au	7.927415000000001	3.162669000000003	7.730100000000004
Au	3.499980000000002	0.606528000000001	7.730100000000004
Au	0.548432999999997	0.606497999999998	7.730100000000004
Au	6.451580000000001	5.718850000000002	7.730100000000004
Au	2.024233000000001	3.162658000000001	7.730100000000004
Au	10.879007000000000	4.866780000000002	5.320100000000003
Au	4.975827000000000	4.866769000000000	5.320100000000003
Au	6.451574000000000	2.310639000000000	5.320100000000003
Au	9.403208000000002	2.310618999999998	5.320100000000003
Au	7.927374000000002	4.866799999999998	5.320100000000003
Au	3.500026999999999	2.310608000000002	5.320100000000003
Au	12.354809000000002	7.422941000000000	5.320100000000003
Au	9.403173000000000	7.422960000000001	5.320100000000003
Au	6.451627000000002	7.422929999999998	5.320100000000003
5.6 pt3_au_6layers-h_au-site1			
H	7.899328999999997	3.178050999999998	18.197796000000000
Pt	10.730929000000000	4.967597000000002	19.412041000000007
Pt	8.104826000000001	4.968481000000001	19.415886000000006
Pt	9.416041000000002	7.243631999999998	19.411572999999990
Au	7.894982000000000	1.480673000000001	17.490356000000004
Au	10.999721999999999	6.642285000000001	17.265833000000001
Au	4.980149000000000	6.528107999999999	17.491215000000001
Au	6.412406999999998	3.989981999999999	17.494616999999996
Au	9.410735000000000	3.881795000000001	17.270904999999989
Au	4.989079000000002	1.528162000000003	17.492200999999990
Au	2.080674999999998	1.493031000000001	17.484158000000006
Au	7.815065999999998	6.644526000000001	17.271133000000006
Au	3.566448999999999	3.992245999999997	17.491960999999990
Au	6.450537000000000	0.619267000000000	14.959823999999991
Au	9.401274000000002	5.716672999999999	14.940660000000001
Au	3.510129000000001	5.712156999999999	14.960968000000008
Au	4.976863000000003	3.163841000000002	14.993640999999996
Au	7.916943999999998	3.151528999999998	14.965238000000003
Au	3.497427000000000	0.619596000000000	14.960077999999997
Au	0.546158000000000	0.602034999999999	14.946261999999990
Au	6.439107999999998	5.711816999999998	14.964829999999993
Au	2.033295999999997	3.154315999999998	14.960236000000003
5.7 pt3_au_6layers-h_au-site2			
H	9.429334000000003	2.298051000000003	18.067794999999990
Pt	10.730929000000000	4.967597000000002	19.412041000000007
Pt	8.104826000000001	4.968481000000001	19.415886000000006
Pt	9.416041000000002	7.243631999999998	19.411572999999990
Au	7.894982000000000	1.480673000000001	17.490356000000004
Au	10.999721999999999	6.642285000000001	17.265833000000001
Au	4.980149000000000	6.528107999999999	17.491215000000001
Au	6.412406999999998	3.989981999999999	17.494616999999996
Au	9.410735000000000	3.881795000000001	17.270904999999989
Au	4.989079000000002	1.528162000000003	17.492200999999990
Au	2.080674999999998	1.493031000000001	17.484158000000006
Au	7.815065999999998	6.644526000000001	17.271133000000006
Au	3.566448999999999	3.992245999999997	17.491960999999990
Au	6.450537000000000	0.619267000000000	14.959823999999991
Au	9.401274000000002	5.716672999999999	14.940660000000001
Au	3.510129000000001	5.712156999999999	14.960968000000008
Au	4.976863000000003	3.163841000000002	14.993640999999996
Au	7.916943999999998	3.151528999999998	14.965238000000003
Au	3.497427000000000	0.619596000000000	14.960077999999997
Au	0.546158000000000	0.602034999999999	14.946261999999990
Au	6.439107999999998	5.711816999999998	14.964829999999993
Au	2.033295999999997	3.154315999999998	14.960236000000003
5.8 pt3_au_6layers-h_au-site3			
H	0.56590796323150	0.61332237526424	18.20014151593645
Pt	10.73092938415266	4.96759727790484	19.41203987331100
Pt	8.10482626197847	4.96848085999555	19.41588673575558
Pt	9.41604144097281	7.24363195924373	19.41157344394058
Au	7.89498173331652	1.48067310832581	17.49035564308764
Au	10.99972192088047	6.64228481533600	17.26583340684090
Au	4.98014902601011	6.52810751932434	17.49121532657149

Au	6.41240754966295	3.98998193707230	17.49461728180268
Au	9.41073552606751	3.88179467723953	17.27090383388303
Au	4.98907969395572	1.52816239873462	17.49220006256284
Au	2.08067517170661	1.49303088758520	17.48415736889414
Au	7.81506615757662	6.64452531870375	17.27113258909416
Au	3.56644875271012	3.99224591184331	17.49195967297657
Au	6.45053677964886	0.61926707296784	14.95982333031913
Au	9.40127328971757	5.71667289107746	14.94066008819862
Au	3.51012914671098	5.71215708083383	14.96096800582189
Au	4.97686334020806	3.16384104528716	14.99364118871697
Au	7.91694409133448	3.15152919999544	14.96523776186448
Au	3.49742677638479	0.61959591627626	14.96007808864135
Au	0.54615755462613	0.60203478466757	14.94626231760073
Au	6.43910804152325	5.71181691940924	14.96482993981499
Au	2.03329641098149	3.15431570434180	14.96023570089287
5.9	<i>pt3_au4x4</i>		
Pt	10.33339954978684	7.07989515593238	12.05995337901622
Pt	11.66068147080884	4.78046330465107	12.06035551156757
Pt	9.00624590098057	4.78123540704100	12.06084793713458
Au	7.27249155659041	3.77883446011288	10.22922196688863
Au	2.96161858528647	1.28933914048070	10.12294093084441
Au	5.89391857417557	1.28982406089364	10.12295004296325
Au	4.42839256843698	3.82784825710181	10.12390572097793
Au	13.39227665473753	3.77731165599253	10.22782418508585
Au	8.81707633497279	1.22650583165542	10.10758248154838
Au	11.84414498896425	1.22498895036948	10.10651626256431
Au	10.33244067180777	3.61042110070883	9.99978635872088
Au	10.33143674749017	9.07853277579356	10.22289751627758
Au	5.83438271654662	6.39450915260971	10.10661275170319
Au	8.65517493123543	6.51360924827520	9.99904916307965
Au	7.34600263463168	9.01520787153586	10.10920110431326
Au	16.23486208693734	8.95243497325002	10.08335012953826
Au	12.00828293393242	6.51249263087418	9.99790217057858
Au	14.82856757484640	6.39394895520929	10.10653632263761
Au	13.31603128062269	9.01494584219393	10.10890658929928
Au	5.90445472888660	2.98787941852107	7.70143429953141
Au	1.47965334747620	0.43261325392379	7.67392306269532
Au	4.42737317658398	0.43269595485389	7.69956550057512
Au	2.95168706133857	2.98670542168420	7.70118486246480
Au	11.82946555968559	2.99255897115438	7.69161622215539
Au	7.37476628399838	0.43365943374901	7.67393328149157
Au	10.33069016088382	0.44194525358192	7.68918697927654
Au	8.83441927141149	2.99321695950810	7.69168323310176
Au	8.87154580196647	8.11672141407730	7.69086302690509
Au	4.42767823892494	5.53809720318459	7.67411398617899
Au	7.37471397921299	5.51972938990773	7.69125951244957
Au	5.91303076695653	8.09440419824218	7.68819828878198
Au	14.74910616487530	8.09473004494606	7.68864642307214
Au	10.33143955018954	5.54414999801277	7.72920161101894
Au	13.28893959112865	5.51875069876709	7.69076753961614
Au	11.79155966339571	8.11679572883275	7.69023775155638
Au	1.47501300000001	2.13410900000003	5.32007399999992
Au	4.42740800000006	2.13410900000003	5.32007399999992
Au	2.95081499999996	4.69027800000000	5.32007399999992
Au	5.90321000000001	4.69027800000000	5.32007399999992
Au	7.37900300000001	2.13410900000003	5.32007399999992
Au	10.33139800000006	2.13410900000003	5.32007399999992
Au	8.85480499999997	4.69027800000000	5.32007399999992
Au	11.80719899999996	4.69027800000000	5.32007399999992
Au	4.42701299999997	7.24710900000000	5.32007399999992
Au	7.37940800000002	7.24710900000000	5.32007399999992
Au	5.90281500000005	9.80327800000004	5.32007399999992
Au	8.85521000000001	9.80327800000004	5.32007399999992
Au	10.33100299999997	7.24710900000000	5.32007399999992
Au	13.28339800000002	7.24710900000000	5.32007399999992
Au	11.80680500000005	9.80327800000004	5.32007399999992
Au	14.75919800000000	9.80327800000004	5.32007399999992
Au	7.37901299999998	3.83821900000001	2.91009800000009
Au	2.95160500000001	1.28205400000000	2.91009800000009

Au	5.90321000000003	1.28205400000000	2.91009800000009
Au	4.42740700000000	3.83821900000001	2.91009800000009
Au	13.28300299999998	3.83821900000001	2.91009800000009
Au	8.85559500000001	1.28205400000000	2.91009800000009
Au	11.80719899999998	1.28205400000000	2.91009800000009
Au	10.33139600000003	3.83821900000001	2.91009800000009
Au	10.33101300000002	8.95121899999998	2.91009800000009
Au	5.90360499999997	6.39505399999997	2.91009800000009
Au	8.85520999999999	6.39505399999997	2.91009800000009
Au	7.37940699999995	8.95121899999998	2.91009800000009
Au	16.23500300000002	8.95121899999998	2.91009800000009
Au	11.80759400000001	6.39505399999997	2.91009800000009
Au	14.75919799999997	6.39505399999997	2.91009800000009
Au	13.28339599999999	8.95121899999998	2.91009800000009
<i>5.10 pt3_au4x4-h_au-site1</i>			
H	8.79938999999998	2.97965800000000	10.92196966339291
Pt	10.48461339973912	7.24479406483084	12.05727097886177
Pt	11.74659249937634	4.92527181314406	12.13523977670506
Pt	9.10365697307389	4.99202930306157	11.93703689211915
Au	7.14766019819801	3.84118880155906	10.47951463189782
Au	2.94147476195548	1.35466918008734	10.11600601436038
Au	5.89410810335416	1.33494820672396	10.11076690758730
Au	4.38859183811982	3.86400675716627	10.11839541833858
Au	13.37167652254271	3.81783448088800	10.24584193353037
Au	8.82757562193861	1.24012814283976	10.09414628467377
Au	11.82450563813532	1.25122275697234	10.08182615517956
Au	10.43556398343691	3.67207909917956	10.01324402421131
Au	10.33281805122662	9.17548479857087	10.16640132677919
Au	5.88660734476299	6.40757040152497	10.11470420870210
Au	8.72724636608937	6.72305973274366	9.95769536194231
Au	7.31039958540604	9.09935659393704	10.07864241759030
Au	16.22113772203425	8.95033181581152	10.05490906316663
Au	12.00911789355695	6.51171049674475	9.94143846427552
Au	14.84822951738822	6.40694741856763	10.09793126418663
Au	13.31195066873536	9.02465467384258	10.08830985728778
Au	5.94251385306744	3.02437764353695	7.72790643092522
Au	1.47461121014096	0.46922735237363	7.65532682110435
Au	4.44352923266166	0.48896057482589	7.68551513086398
Au	2.94956131669544	3.01042643821607	7.69473587329111
Au	11.81671694411474	3.00721748516129	7.68283544439826
Au	7.37617466293767	0.45272186298733	7.67253609346733
Au	10.32078185302902	0.43866026636218	7.67862505796992
Au	8.84800589477054	3.01314199480955	7.69309789577027
Au	8.86995086960372	8.18750702984115	7.63340412280231
Au	4.45253145121693	5.54111209282237	7.67329930907672
Au	7.40512796075120	5.52683606596068	7.73121093789055
Au	5.91895211701873	8.08563928063187	7.68683381289063
Au	14.74556439301590	8.08478836729306	7.67980501539976
Au	10.31864922942036	5.55798373820305	7.72913879483101
Au	13.30430041674963	5.52357498766063	7.67540161502326
Au	11.78685547399702	8.13407101872892	7.67366524204621
<i>5.11 pt3_au4x4-h_au-site2</i>			
H	10.36940200000000	2.12965900000002	10.85391596243195
Pt	10.33403924971693	7.10157525435173	12.05003173934953
Pt	11.66383130947626	4.82184442227075	12.09992030382532
Pt	9.01099806611463	4.81849555839927	12.10632478162987
Au	7.27451768238875	3.80495335686077	10.24785289565135
Au	2.96028831541271	1.29957836797551	10.10462479980046
Au	5.91034186988614	1.30188187095024	10.10558990417508
Au	4.43183018062900	3.82517906567844	10.12849555296895
Au	13.39788126136476	3.80520926324277	10.24108036106715
Au	8.82135039906182	1.24358337253170	10.18654971323489
Au	11.86616185960340	1.23607866109988	10.18862609594086
Au	10.33462918219075	3.78102657424085	9.94508385069174
Au	10.33882933359901	9.09342160163139	10.21153270955818
Au	5.83698409122566	6.39335085130356	10.10839366722736
Au	8.65698723673213	6.51473930244147	9.99362201761007
Au	7.35838524272163	9.02156019493103	10.09094676857135
Au	16.23857173755679	8.94528194872434	10.06158701848899

Au	12.01363234100291	6.52323635875594	9.99300161167986
Au	14.83250980599403	6.39364389858428	10.10866056949384
Au	13.31673309137105	9.03110175444628	10.09335683108780
Au	5.90396782062532	2.98835156143143	7.70519547779777
Au	1.45950685592306	0.44906569784708	7.68620968809795
Au	4.42983861956115	0.43251139157346	7.68759708314445
Au	2.95368542675334	2.98696436437968	7.70430335226854
Au	11.83503733839410	2.99609129356734	7.68838215899522
Au	7.40018592171197	0.45170155417504	7.68640324411609
Au	10.33318374502661	0.44691871904423	7.69241153053587
Au	8.83117412629428	2.99635304398518	7.68904879133392
Au	8.87222078418941	8.12828505717236	7.68616328144824
Au	4.42834186513907	5.53415665494945	7.67428872456443
Au	7.36897970686757	5.52686292152250	7.69088081426912
Au	5.91494428564060	8.09567849347493	7.68858619610123
Au	14.74952269388447	8.09567105003581	7.68914230369590
Au	10.33307364873380	5.56114463360687	7.70824874027867
Au	13.29580367357702	5.52794604810932	7.69040091836985
Au	11.79401592255651	8.13165296913102	7.68591154202869
<i>5.12 pt3_au4x4-h_au-site3</i>			
H	4.42682275333615	7.23914539761436	11.00112717915295
Pt	10.33168980188240	7.08499627060560	12.06178941474459
Pt	11.65941974352458	4.78466117305851	12.05426728496032
Pt	9.00625072246110	4.78364836859867	12.05502965107270
Au	7.27717280224193	3.76680871446225	10.22401527361454
Au	2.95868786954351	1.28013495162715	10.13112737023754
Au	5.89575526911222	1.28103432688986	10.13179004902243
Au	4.42724734932950	3.79403450152133	10.10219214806465
Au	13.38581318517787	3.76479161964920	10.22261624017651
Au	8.82187347958152	1.23819118741231	10.10216584157754
Au	11.83973215845879	1.23763805721292	10.10090633733751
Au	10.33150522540401	3.63409128393640	9.98402585218156
Au	10.33149915446174	9.07442055490891	10.21998256291987
Au	5.86961512248619	6.35437105134450	10.20753053828955
Au	8.65998651123306	6.51129273091540	9.99634902894830
Au	7.35726984789049	9.02442438846447	10.08441169362234
Au	16.23535358045867	8.99292706968845	10.16069384011301
Au	12.00194091374259	6.51163388903084	9.99494639933130
Au	14.79222017219323	6.35372114525269	10.20765290649868
Au	13.30481766848243	9.02455526201584	10.08517008213501
Au	5.90570175937299	2.98240343038448	7.70169888704106
Au	1.47734125108769	0.43867543520338	7.67252571996138
Au	4.42737740402556	0.42855505811941	7.70248325915604
Au	2.94961153715201	2.98239040030630	7.70116581829784
Au	11.82520160693518	2.99467266646378	7.68272651391774
Au	7.37650244810048	0.43855421144875	7.67260852436254
Au	10.32994954923383	0.41011590742600	7.70722835462954
Au	8.83716601509336	2.99478246215150	7.68313053254023
Au	8.86941414504136	8.11216539877857	7.68998494797984
Au	4.42745770213584	5.53901579610386	7.68659836851479
Au	7.34344937187033	5.52920626390443	7.71468128585520
Au	5.90613436371796	8.09053521796027	7.69729343918382
Au	14.75664051427727	8.09017165612947	7.69717785152086
Au	10.33115301798554	5.54188004960000	7.71180949721861
Au	13.31882463571017	5.52817179349313	7.71445145137029
Au	11.79444701082949	8.11206072818263	7.68931880140717